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Institut für Kristallographie der RWTH Aachen
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Institut für Festkörperforschung der KFA Jülich

UNISOFT –

A PROGRAM PACKAGE FOR LATTICE-DYNAMICAL CALCULATIONS: USER MANUAL

by

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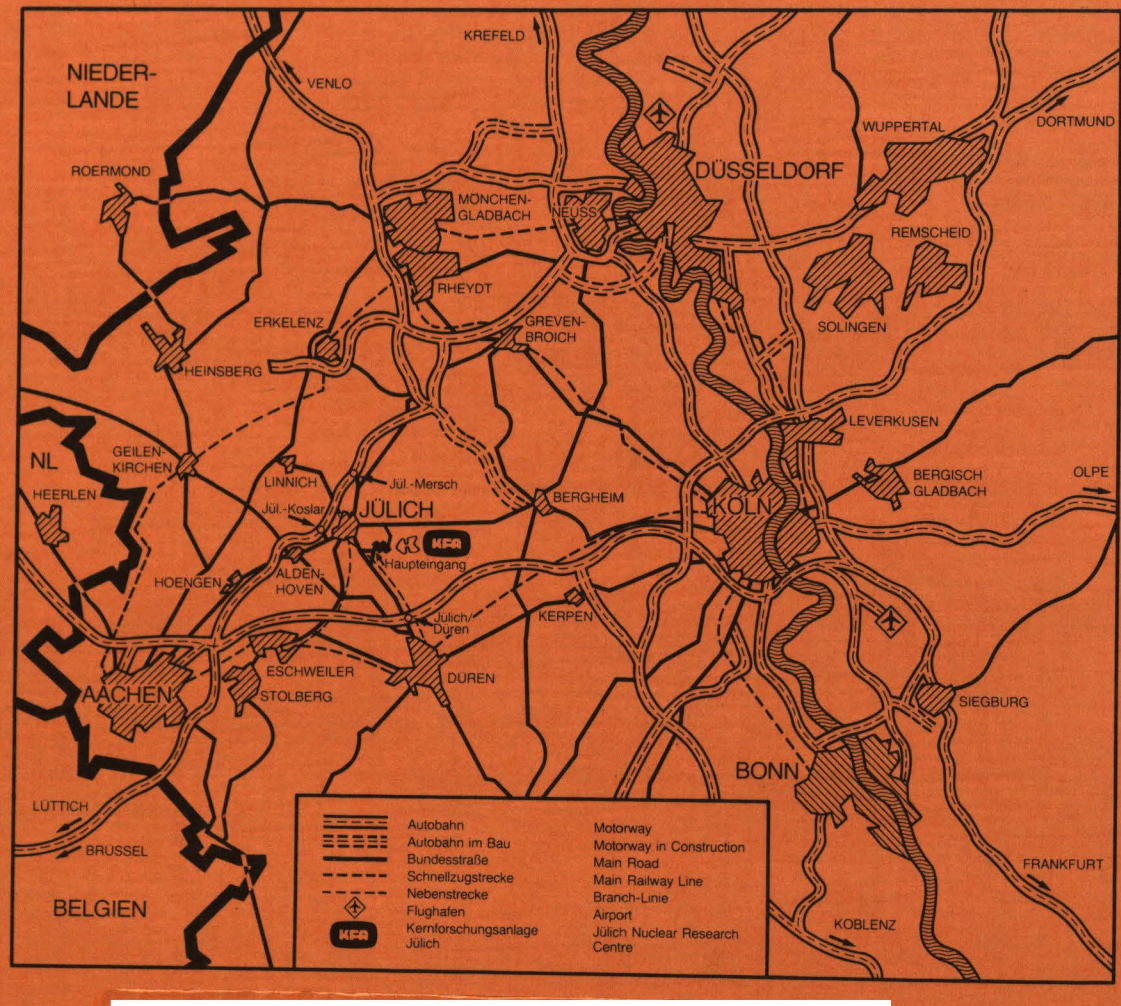

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1.0 Introduction

Lattice-dynamical investigations provide a powerful tool for the determination of interatomic forces and chemical bonding in crystals. In general the extraction of, say, potential parameters from phonon dispersion curves, as determined experimentally, is possible with the help of model calculations only. Phonons which are cooperative excitations in many-body systems provide informations about interactions within the whole crystal. A quantitative interpretation of single phonons is therefore restricted to very simple crystal structures. In general, however, unambigious statements about interatomic forces require the knowledge of a good number of the phonon branches, at least in the symmetry directions.

Often, the determination of phonon dispersion curves is a rather hard task since a crystal with N particles per unit cell exhibits as many as 3N phonon branches. The only experimental method which allows the detection of phonons at arbitrary points within the Brillouin zone is the inelastic neutron scattering. Again, model calculations are very useful and sometimes even necessary in order to find phonons experimentally since phonon intensities vary strongly from one Brillouin zone to another and are determined by the corresponding eigenvectors. For complex structures, model calculations and neutron scattering experiments are thus complementary. The determination of interatomic forces in crystals requires both, the theoretical and the experimental approach which need to go hand in hand.

The three-axes spectrometer UNIDAS at the FRJ-2 reactor at Jülich is available to external users and is especially designed to meet the requirements for phonon investigations. Details of this machine are described in the UNIDAS-Handbuch [1]. In the present paper we report on the complement to this spectrometer, namely the computer program package UNISOFT which allows to perform model calculations on phonon dispersion in general structures with up to 20 particles per primitive cell.

UNISOFT has been developed in order to provide a tool for the optimization of experiments as well as for a first interpretation of the results. Certainly, a general lattice-dynamical program cannot deal with the most complex models for interatomic interactions. Until now the standard models such as

- Born-von Karman model (longitudinal and transverse springs)
- Born-Mayer potential
- Lennard-Jones potential
- van der Waals potential
- Coulomb potential (Ewald's method of summation)
- shell model

are implemented. The interaction between each pair of atoms can be chosen individually as an arbitrary combination of these model potentials. More sophisticated models must be developed by the user and are beyond the scope of UNISOFT as a universally applicable lattice-dynamical program.

Special attention has been paid to the handling of this program package by external users. Offering the possibility of a tailored interatomic interaction set-up for each individual substance under consideration, the system is rather complex, of course. Universality of the programs, however, does not exclude an easy mode of operation. Thus, UNISOFT can indeed be used in combination with UNIDAS by experimenters which are not familiar with details of lattice-dynamical calculations and the interpretation of phonon dispersion curves. This combination of software and hardware is able to simplify the determination of interatomic forces in crystals even for non-specialists.

Chapter 2 of this report briefly reviews the theoretical background of lattice dynamics in the harmonic approximation along with group-theoretical considerations and symmetry constraints to the dynamical matrix. The response of a phonon system in neutron scattering experiments is also discussed. In section 3 the global structure of the program package is displayed before a detailed description of the individual programs is given in chapter 4. Section 5 deals with computer requirements. Some possible extensions of this program system are discussed in chapter 6. In order to illustrate all information available with UNISOFT, an example for a complete treatment of a crystal structure within this program system is presented in appendix A. Finally, a comprehensive list of all input cards, the alphabetical list of subroutines, the subroutine reference list and the list of symbols used in this manual are given in the appendices B, C, D and E.

Concerning the notation, matrices are denoted by bold printed capital letters and vectors are represented by bold printed lower case letters.

2.0 Fundamentals of Lattice Dynamics

In this chapter we give a brief summary of the theoretical basis used for lattice-dynamical calculations. For a detailed treatment the reader is referred to the review articles by *LEIBFRIED* [2], *COCHRAN* and *COWLEY* [3], *MARADUDIN* and *VOSKO* [4] and the references therein.

2.1 Lattice Dynamics in the Harmonic Approximation

Lattice dynamics in the harmonic approximation describes the modes of motion in a crystalline solid in the case of small displacements of the atoms from their respective equilibrium positions. If there are N particles per primitive cell and N_c cells per crystal the (time-dependent) position of the κ-th atom ($\kappa = 1 \ldots N$) within the l-th primitive cell ($l = 1 \ldots N_c$) is given by

$$\mathbf{r}_{\kappa l}(t) = \mathbf{r}_\kappa + \mathbf{r}_l \,. \tag{2.1}$$

$\mathbf{r}_l$ is the vector to the origin of the l-th cell. $\mathbf{r}^o_{\kappa l}$ and $\mathbf{r}^o_\kappa$ denote the corresponding equilibrium values. The displacement of atom (κl) is thus:

$$\mathbf{u}_{\kappa l}(t) = \mathbf{r}_{\kappa l}(t) - \mathbf{r}^o_{\kappa l} \,. \tag{2.2}$$

The Hamiltonian for this crystal system may be represented by

$$H = \sum_{\kappa\, l}\sum \frac{\mathbf{p}^2_{\kappa l}}{2m_\kappa} + \sum_{\kappa\, l\, \kappa' l'}\sum\sum\sum V(\kappa l, \kappa' l') \,, \tag{2.3}$$

m_κ and $\mathbf{p}_{\kappa l}$ being the mass and the momentum of particle (κl), respectively. $V(\kappa l, \kappa' l')$ is the interaction potential between particles (κl) and ($\kappa' l'$). Three-body forces and higher-order interactions are neglected. In equilibrium the second term in equation (2.3) takes the constant value V_o. If only small displacements of the atoms from their equilibrium positions are considered the potential energy may be expanded in powers of $\mathbf{u}_{\kappa l}$. Retaining the terms up to the second order in the displacements and dropping the constant V_o one obtains for the Hamiltonian:

$$H = \frac{1}{2}\sum_{\kappa\, l}\sum m_\kappa \dot{\mathbf{u}}^2_{\kappa l} + \frac{1}{2}\sum_{\kappa\, l\, \kappa' l'}\sum\sum\sum \mathbf{u}_{\kappa l} V(\kappa l, \kappa' l') \mathbf{u}_{\kappa' l'} \,. \tag{2.4}$$

All first-order terms vanish since the potential energy is minimized in the equilibrium position. For $(\kappa l) \neq (\kappa' l')$, $V(\kappa l, \kappa' l')$ is the matrix of second derivatives of the pair potential $V(\kappa l, \kappa' l')$ taken at the equilibrium positions:

$$V_{\alpha\beta}(\kappa l, \kappa' l') = - \frac{\partial^2 V(\kappa l, \kappa' l')}{\partial r_\alpha \partial r_\beta}\Big|_{\mathbf{r} = \mathbf{r}^o_{\kappa' l'} - \mathbf{r}^o_{\kappa l}} \,. \tag{2.5}$$

$-V(\kappa l, \kappa' l')\, \mathbf{u}_{\kappa' l'}$ is the force acting upon the atom (κl) when ($\kappa' l'$) is displaced by $\mathbf{u}_{\kappa' l'}$. Thus V is a force constant matrix. The self term $V(\kappa l, \kappa l)$ describes the restoring force if only atom (κl) is displaced and all the other atoms are at rest. $V(\kappa l, \kappa l)$ is *not* the second-derivative matrix of a self potential but is given by:

$$V(\kappa l, \kappa l) = - \sum_{(\kappa' l') \neq (\kappa l)} V(\kappa l, \kappa' l') \,. \tag{2.6}$$

Equation (2.6) is a consequence of the fact that there cannot be a force on any atom if the crystal as a whole is translated. From equation (2.4) one obtains the equations of motion:

$$m_\kappa \ddot{\mathbf{u}}_{\kappa l} = - \sum_{\kappa' l'}\sum V(\kappa l, \kappa' l')\, \mathbf{u}_{\kappa' l'} \,. \tag{2.7}$$

Solutions of this set of coupled differential equations are of the form:

$$\mathbf{u}_{\pm}(\kappa l \mid qj) = \frac{1}{\sqrt{Nm_\kappa}} e(\kappa \mid qj)\, e^{i(\mathbf{q}\mathbf{r}_l \pm \omega_{qj} t)} \tag{2.8}$$

which are plane waves with wave vector $\mathbf{q}$ and polarization vector $e(\kappa \mid qj)$. Due to periodic boundary conditions $\mathbf{q}$ is restricted to a sequence of discrete values which, however, are very close to each other. Thus, for practical work $\mathbf{q}$ can be treated as a continuous variable. For each $\mathbf{q}$ there are 3N different modes of vibration or *phonons* represented by different polarization vectors $e(\kappa \mid qj)$ and frequencies ω_{qj} $(j = 1 \ldots 3N)$. The actual displacement of the atom (κl) is a linear combination

$$\mathbf{u}_{\kappa l} = \sum_{q} \sum_{j} [A_{qj}\mathbf{u}_{+}(\kappa l \mid qj) + A'_{qj}\mathbf{u}_{-}(\kappa l \mid qj)] . \tag{2.9}$$

Since $\mathbf{u}(\kappa l)$ is a real vector equation (2.9) can be transformed into:

$$\mathbf{u}_{\kappa l} = \frac{1}{\sqrt{Nm_\kappa}} \sum_{q} \sum_{j} Q_{qj} e(\kappa \mid qj)\, e^{i\mathbf{q}\mathbf{r}_l} \tag{2.10}$$

where

$$Q_{qj} = A_{qj} e^{-i\omega_{qj} t} + A^{*}_{-qj} e^{i\omega_{qj} t} \tag{2.11}$$

are the *Normal Coordinates.* * denotes the complex conjugate. These normal coordinates determine the amplitude of the lattice vibrations or, in other words, the number of phonons which are excited at a given temperature. The average values may be calculated by statistical methods (see section 2.7).

The Hamiltonian (2.4) can be expressed in terms of the normal coordinates as:

$$H = \frac{1}{2N} \sum_{q} \sum_{j} [|\dot{Q}_{qj}|^2 + \omega_{qj} |Q_{qj}|^2] \tag{2.12}$$

which is just the superposition of the Hamiltonians of 3N independent harmonic oscillators for each $\mathbf{q}$.

The polarization vectors $e(\kappa \mid qj)$ and the frequencies ω_{qj} are obtained as eigenvectors and eigenfrequencies of the Fourier transformed force constant matrix multiplied by the square root of the masses:

The (3×3) submatrices

$$\mathbf{D}(\kappa\kappa' \mid q) = \frac{1}{\sqrt{m_\kappa m_{\kappa'}}} \sum_{l'} V(\kappa l, \kappa' l') e^{iq(\mathbf{r}_{l'} - \mathbf{r}_l)} \tag{2.13}$$

are assembled within a $(3N \times 3N)$ matrix:

$$\mathbf{D}(q) = \begin{pmatrix} \mathbf{D}(11 \mid q) & \cdots & \mathbf{D}(1N \mid q) \\ \vdots & & \vdots \\ \mathbf{D}(N1 \mid q) & \cdots & \mathbf{D}(NN \mid q) \end{pmatrix} \tag{2.14}$$

which is called the *Dynamical Matrix.*[1] It should be noticed that the right hand side of equation (2.13) is independent of l since only the differences $\mathbf{r}_{l'} - \mathbf{r}_l$ enter in $V(\kappa l, \kappa' l')$ as well as in the phase factor.

Collecting the polarization vectors $e(\kappa \mid qj)$ in an analogous manner:

$$e(qj) = \begin{pmatrix} e(1 \mid qj) \\ \vdots \\ e(N \mid qj) \end{pmatrix} \tag{2.15}$$

it can immediately be seen from equation (7) that the following eigenvector equation holds:

$$\omega_{qj}^2\, e(qj) = \mathbf{D}(q)\ e(qj) . \tag{2.16}$$

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[1] This is the D-definition of the Dynamical Matrix in the notation of *MARADUDIN* and *VOSKO* [4]. Another definition, the C-definition, is obtained if the phase factors $e^{iq(r^0_{\kappa'} - r^0_{\kappa})}$ are included.

Usually, the eigenvectors e(qj) are chosen to be orthonormalized and to have the property:

$$\mathbf{e}^{*}(\mathbf{qj}) = \mathbf{e}(-\mathbf{qj}) . \tag{2.17}$$

Once the Dynamical Matrix is known, the displacement pattern and the frequency of each of the 3N phonons can be calculated. Inspection of the definition, equation (9), leads to the fact that **D** must be hermitian and, consequently, the eigenvalues ω^2 are real quantities.

For later use it is convenient to introduce the notation **F(q)** for the Fourier transformed force constant matrix which is built from the (3×3) submatrices $\mathbf{F}(\kappa\kappa' | \mathbf{q})$ in the same way as **D(q)** is built from $\mathbf{D}(\kappa\kappa' | \mathbf{q})$:

$$\mathbf{F}(\kappa\kappa' | \mathbf{q}) = \sum_{l'} \mathbf{V}(\kappa l, \kappa' l') e^{i\mathbf{q}(\mathbf{r}_{l'} - \mathbf{r}_{l})} . \tag{2.18}$$

The Dynamical Matrix can now be expressed as:

$$\mathbf{D(q)} = \mathbf{M}\ \mathbf{F(q)}\ \mathbf{M} \tag{2.19}$$

where **M** is the diagonal matrix of the inverse square roots of the atomic masses:

$$M_{\alpha\beta}(\kappa\kappa') = \frac{1}{\sqrt{m_{\kappa}}} \delta_{\alpha\beta}\delta_{\kappa\kappa'} . \tag{2.20}$$

Modelling the vibrational properties of a crystal within the harmonic approximation obviously implies the construction of the Dynamical Matrix. There are several approaches which are commonly used:

1. The force constants, *i.e.* the elements of $V(\kappa l,\kappa' l')$, are used as adjustable parameters directly. Known as the *Born-von Karman model*, this approach is suitable only for cases in which short range forces dominate. Otherwise the number of model parameters becomes too large.

2. Interatomic potentials are put forward and the force constants are calculated as second derivatives of these model potentials according to equation (2.5). In the case of long-range potentials, such as the Coulomb potential, special tricks are needed in order to overcome the problem of slow convergence of the Fourier series in equation (2.13) (Ewald-summation [5] or Bertaut-approach [6]).

3. Other degrees of freedom such as the motion of electron shells may be introduced in order to simulate electrical polarization effects.

More complicated and sometimes sophisticated models have been devised for special crystals. Here, however, we restrict ourselves to rather simple interatomic force models which are applicable as standard models to a variety of different materials and which, therefore, are suitable for the use in a general lattice-dynamical program like UNISOFT. It should be mentioned, however, that even on the basis of a few simple interatomic interaction types a rather complex model set-up can be generated simply by combining two or more of these types.

In the following, the three principal approaches for the construction of the Dynamical Matrix are discussed in some detail.

2.2 *Born-von Karman model*

In the Born-von Karman model the force constants are treated as model parameters. They are *not* interpreted in terms of a special interatomic potential. Due to the symmetry of the force constant matrix each interaction is described by six force constants:

$$\mathbf{V}(\kappa l, \kappa' l') = \begin{pmatrix} a & b & c \\ b & d & e \\ c & e & f \end{pmatrix} . \tag{2.21}$$

Assuming the forces to be central forces, the number of parameters is reduced to two, namely the

Longitudinal Force Constant

$$L = \frac{d^2 V(\kappa l, \kappa' l')}{dr^2}\Big|_{r = |\mathbf{r}^{0}_{\kappa' l'} - \mathbf{r}^{0}_{\kappa l}|} \tag{2.22}$$

and the

Transverse Force Constant

$$T = \frac{1}{r}\frac{dV(\kappa l, \kappa' l')}{dr}\Big|_{r=|r^0_{\kappa' l'} - r^0_{\kappa l}|} . \tag{2.23}$$

In terms of these parameters the elements of $V(\kappa l, \kappa' l')$ are:

$$V_{\alpha\beta}(\kappa l, \kappa' l') = (L - T)\frac{r_\alpha r_\beta}{r^2} + T\ \delta_{\alpha\beta} \tag{2.24}$$

where r_α is the cartesian component of $\mathbf{r} = \mathbf{r}^0_{\kappa' l'} - \mathbf{r}^0_{\kappa l}$ in direction α and r is the modulus of $\mathbf{r}$.

Obviously, this description of interatomic forces is restricted to short-range interactions. These interactions can be visualized by springs. L corresponds to the ordinary longitudinal spring producing restoring forces if the distance between the atoms (κl) and $(\kappa' l')$ is altered. T, on the other hand, corresponds to a transverse spring producing restoring forces if one atom is displaced in a direction perpendicular to the bond.

2.3 *Explicit Interatomic Potentials*

If two types of atoms κ and κ' are coupled via a potential which can be formulated explicitly and which is valid over a certain range of interatomic distances then the force constants for all pairs (κl) and $(\kappa' l')$ can be calculated from this potential. In this case, the number of parameters is reduced and long-range interactions such as Coulomb forces are feasible. Several model potentials are commonly used and included in UNISOFT:

BORN-MAYER:

$$V_{\kappa\kappa'}(r) = V_0 \exp\left(-\frac{r}{\sigma_\kappa + \sigma_{\kappa'}}\right) \tag{2.25}$$

$$L = \frac{V_0}{(\sigma_\kappa + \sigma_{\kappa'})^2}\exp\left(-\frac{r}{\sigma_\kappa + \sigma_{\kappa'}}\right) \tag{2.26}$$

$$T = -\frac{V_0}{(\sigma_\kappa + \sigma_{\kappa'})r}\exp\left(-\frac{r}{\sigma_\kappa + \sigma_{\kappa'}}\right) \tag{2.27}$$

LENNARD-JONES:

$$V_{\kappa\kappa'}(r) = V_0\left[\left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^{12} - \left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^{6}\right] \tag{2.28}$$

$$L = 6\frac{V_0}{r^2}\left[26\left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^{12} - 7\left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^{6}\right] \tag{2.29}$$

$$T = -6\frac{V_0}{r^2}\left[2\left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^{12} - \left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^{6}\right] \tag{2.30}$$

van der WAALS:

$$V_{\kappa\kappa'}(r) = -V_0\left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^{6} \tag{2.31}$$

$$L = -42\frac{V_0}{r^2}\left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^{6} \tag{2.32}$$

$$T = 6\frac{V_0}{r^2}\left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^{6} \tag{2.33}$$

COULOMB:

$$V_{\kappa\kappa'} = \frac{Z_\kappa Z_{\kappa'}}{4\pi\varepsilon_0 r} . \tag{2.34}$$

The first three potentials are short ranged and the Dynamical Matrix can be calculated by direct summation according to equation (2.13). The Coulomb interaction, however, requires a special treatment since the series in equation (2.13) is non-convergent due to the fact that we are dealing with point charges. Replacing the point charges by charge distributions, however, the Fourier transform of the second derivatives of this potential can be given explicitly. For a Gaussian charge distribution, *e.g.*,

$$\rho_\kappa = Z_\kappa \sqrt{\frac{p}{\pi}}^3 e^{-pr^2} \tag{2.35}$$

as introduced by *EWALD* [5], the Fourier transform of the second derivatives is:

$$F^G_{\alpha\beta}(\kappa\kappa'|q) = \frac{Z_\kappa Z_{\kappa'}}{\varepsilon_0 V} \sum_g \frac{(g+q)_\alpha (g+q)_\beta}{|g+q|^2} \exp\left[\frac{-|g+q|^2}{4p}\right] \exp\left[ig(r^0_\kappa - r^0_{\kappa'})\right]. \tag{2.36}$$

The summation runs over all reciprocal lattice vectors g and is rapidly convergent due to the Gaussian damping factor. v is the volume of the primitive cell.[2] The overlap of the charge distributions of different atoms requires a correction term taking into account the difference between the potential of point charges and Gaussian charge distributions. This term can be written as:

$$V^{overlap}_{\kappa\kappa'}(r) = 2\sqrt{\frac{p}{\pi}} \frac{Z_\kappa Z_{\kappa'}}{4\pi\varepsilon_0 r} \int_r^\infty e^{-px^2} dx. \tag{2.37}$$

The error function guarantees the corresponding Fourier series of the second derivatives being rapidly convergent in direct space:

$$F^{overlap}_{\alpha\beta}(\kappa\kappa'|q) = -\sum_{l'} \frac{\partial^2 V^{overlap}_{\kappa\kappa'}(r)}{\partial r_\alpha \partial r_\beta} e^{iqr}\Big|_{r = r^0_{\kappa l} - r^0_{\kappa' l'}}. \tag{2.38}$$

The parameter p which determines the width of the Gaussian charge distribution can be adjusted in order to optimize the convergence of both series, in direct and reciprocal space, simultaneously. The entire Coulomb part of the Fourier transformed force constant matrix is the sum:

$$F^C(\kappa\kappa'|q) = F^G(\kappa\kappa'|q) + F^{overlap}(\kappa\kappa'|q). \tag{2.39}$$

The self term corresponding to V(κl, κl) which is *not* the second derivative of the self potential, as pointed out earlier, must be taken into account by:

$$F^C(\kappa\kappa|q) = F^G(\kappa\kappa|q) + F^{overlap}(\kappa\kappa|q) - \sum_{\kappa'} [F^G(\kappa\kappa'|0) + F^{overlap}(\kappa\kappa'|0)]. \tag{2.40}$$

It is convenient to introduce the *matrix of Coulomb coefficients* **C** as:

$$C(\kappa\kappa'|q) = \frac{1}{Z_\kappa Z_{\kappa'}} F^C(\kappa\kappa'|q). \tag{2.41}$$

C is independent of the atomic properties and is entirely determined by the crystal structure. Defining the diagonal matrix of the charges **Z** by:

$$Z_{\alpha\beta}(\kappa\kappa') = Z_\kappa \, \delta_{\alpha\beta}\delta_{\kappa\kappa'} \tag{2.42}$$

and collecting the full (3N × 3N) matrix **C**(**q**) in analogy to equation (2.14), equation (2.41) can be rewritten as:

$$\mathbf{F^C(q) = Z\ C(q)\ Z} \tag{2.43}$$

and the Coulomb part of the Dynamical Matrix is given by:

$$\mathbf{D^C(q) = M\ Z\ C(q)\ Z\ M}. \tag{2.44}$$

Another method to deal with the Coulomb potential has been introduced by *BERTAUT* [6]. Here, the point charges are replaced by charge distributions which, on the one hand, are broad enough to guarantee a rapid convergence of the Fourier series corresponding to equation (2.36), but which, on the other hand, do not overlap. Charge distributions of this kind may be described by

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[2] In numerical calculations q must not be set exactly equal to zero since then the q = 0 term cannot be evaluated. Due to the neglect of retardation effects very long phonon wavelenghts cannot be treated in this way. The Γ-point phonons are approximated in lattice-dynamical calculations by the consideration of small but non-zero wavevectors. The LO-TO-splitting is obtained as the difference of phonon frequencies if the Γ-point is approached from different directions.

polynomials in $|\mathbf{r} - \mathbf{r}^0_{\kappa l}|$ the coefficients of which are determined by the nearest neighbour distances. This method, however, is not used within UNISOFT. Therefore, details of the Bertaut-approach are not given here.

2.4 *Combination of Different Interactions*

Sometimes, a particular interaction between atoms of type κ and κ' is to be described as a superposition of several model potentials m. In this case, the corresponding submatrices $\mathbf{D}(\kappa\kappa'|\mathbf{q})$ and $\mathbf{F}(\kappa\kappa'|\mathbf{q})$ of the Dynamical Matrix and of the Fourier transformed force constant matrix can be calculated as a sum

$$\begin{aligned} \mathbf{D}(\kappa\kappa'|\mathbf{q}) &= \sum_m \mathbf{D}^{(m)}(\kappa\kappa'|\mathbf{q}) \\ \mathbf{F}(\kappa\kappa'|\mathbf{q}) &= \sum_m \mathbf{F}^{(m)}(\kappa\kappa'|\mathbf{q}) \end{aligned} \tag{2.45}$$

where $\mathbf{D}^{(m)}(\kappa\kappa'|\mathbf{q})$ and $\mathbf{F}^{(m)}(\kappa\kappa'|\mathbf{q})$ are entirely determined by the potential m. The interaction between other atoms λ and λ' may be modelled by another combination of potentials. Thus, for each individual crystal a very specific interaction set-up can be provided. The linear combination of the different contributions $\mathbf{D}^{(m)}(\kappa\kappa'|\mathbf{q})$ finally gives the total dynamical matrix $\mathbf{D}(\mathbf{q})$.

The model in which the Coulomb interaction is combined with the short range repulsive Born-Mayer potential for all atoms is known as the *Rigid Ion Model.*

2.5 *Shell Model*

In all models for interatomic interactions discussed so far, the atoms are assumed to be hard spheres. The existence of a deformable electron shell is neglected and, hence, effects due to electronic polarization cannot be accounted for. In a large number of crystals, however, the polarizability plays an important role and a proper lattice-dynamical treatment requires the consideration of the motion of electron shells.

The *shell model* introduced by *DICK* and *OVERHAUSER* [7] provides one of the simplest methods to deal with this problem: Each atom (κl) is divided into a sherically-symmetrical outer electron shell and a core consisting of the nucleus and the inner electrons. If the shell and the core carry the charges Y_κ and X_κ, respectively, the total charge of particle (κl) is given by $Z_\kappa = X_\kappa + Y_\kappa$. In equilibrium, the shell is centered at the position of the corresponding atom core, $\mathbf{r}^0_{\kappa l}$. The shell may be displaced from the core and its momentary position is denoted by $\mathbf{w}_{\kappa l}$. The electric dipole moment of the atom (κl) is thus:

$$\mathbf{p}^e_{\kappa l} = Y_\kappa(\mathbf{w}_{\kappa l} - \mathbf{u}_{\kappa l}) = Y_\kappa \overline{\mathbf{w}}_{\kappa l}\,, \tag{2.46}$$

$\overline{\mathbf{w}}_{\kappa l}$ being the relative displacement of the shell with respect to the core $\overline{\mathbf{w}}_{\kappa l} = \mathbf{w}_{\kappa l} - \mathbf{u}_{\kappa l}$. The electron shell can now be regarded as an additional particle interacting with neighbouring atoms and neighbouring shells. Usually, these interactions are described in terms of the rigid ion model: In addition to their Coulomb interaction, represented by the matrix of second derivatives V^C, shells and cores are considered to be interconnected by (longitudinal and transverse) springs. The direct core-core interactions is treated just as in the preceeding sections. For each two atoms (κl) and (κ'l') the short-range coupling is illustrated schematically in Figure 1 on page 9.
Mathematically, the short-range interactions of the shell model are represented by the force constant matrices $V^{SR}(\kappa l, \kappa' l')$, $V^S(\kappa l, \kappa' l')$, $V^T(\kappa l, \kappa' l')$ and $V^{T'}(\kappa l, \kappa' l')$. V^{SR} is associated with the direct core-core coupling as discussed previously. $V^S(\kappa l, \kappa' l')$ describes the shell-shell interaction. $V^T(\kappa l, \kappa' l')$ is the force constant matrix for the coupling between core(κl) and shell($\kappa' l'$) and $V^{T'}(\kappa l, \kappa' l')$ is the corresponding matrix for the interaction between shell(κl) and core($\kappa' l'$) of different particles (κl) and ($\kappa' l'$). Obviously, the following equation holds:

$$V^T_{\alpha\beta}(\kappa l, \kappa' l') = V^{T'}_{\beta\alpha}(\kappa' l', \kappa l)\,. \tag{2.47}$$

Special attention has to be paid to the the proper consideration of the self terms which are calculated according to equation (2.6):

$$V^T(\kappa l, \kappa l) = - \sum_{(\kappa' l') \neq (\kappa l)} V^T(\kappa l, \kappa' l') \tag{2.48}$$

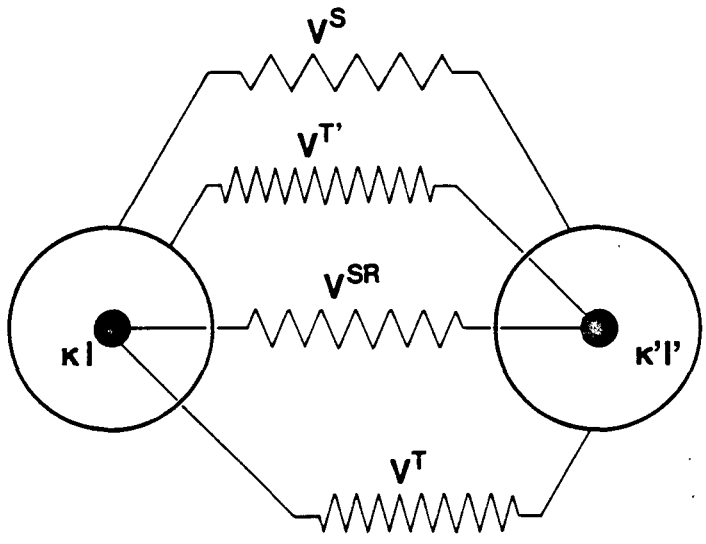

Figure 1. The interactions of two atoms according to the shell model.

$$V^{T'}(\kappa l, \kappa l) = - \sum_{(\kappa' l') \neq (\kappa l)} V^{T'}(\kappa l, \kappa' l') \tag{2.49}$$

$$V^{S}(\kappa l, \kappa l) = - \sum_{(\kappa' l') \neq (\kappa l)} V^{S}(\kappa l, \kappa' l') \; . \tag{2.50}$$

Note that V^T and $V^{T'}$ do not include the coupling between core and shell within the same atom. This interaction is described by an extra force constant K_κ which may be represented by the shell charge Y_κ and the free ion polarizability α_κ:

$$K_\kappa = \frac{Y_\kappa^2}{\alpha_\kappa} \; . \tag{2.51}$$

Collecting all interactions visualized in Figure 1, the following equations of motion are obtained:

For the cores:

$$\begin{aligned} m_\kappa \ddot{u}_{\kappa l} = {} & X_\kappa \sum_{\kappa' l'}\sum V^{C}(\kappa l, \kappa' l')\,[X_{\kappa'} u_{\kappa' l'} + Y_{\kappa'} w_{\kappa' l'}] + \\ & + \sum_{(\kappa' l') \neq (\kappa l)} [V^{SR}(\kappa l, \kappa' l') u_{\kappa' l'} + V^{T}(\kappa l, \kappa' l') w_{\kappa' l'}] + \\ & + K_\kappa w_{\kappa l} + [V^{SR}(\kappa l, \kappa l) + V^{T}(\kappa l, \kappa l) - K_\kappa]\, u_{\kappa l} \end{aligned} \tag{2.52}$$

and for the shells:

$$\begin{aligned} m_s \ddot{w}_{\kappa l} = {} & Y_\kappa \sum_{\kappa' l'}\sum V^{C}(\kappa l, \kappa' l')\,[X_{\kappa'} u_{\kappa' l'} + Y_{\kappa'} w_{\kappa' l'}] + \\ & + \sum_{(\kappa' l') \neq (\kappa l)} [V^{T'}(\kappa l, \kappa' l') u_{\kappa' l'} + V^{S}(\kappa l, \kappa' l') w_{\kappa' l'}] + \\ & + K_\kappa u_{\kappa l} + [V^{T'}(\kappa l, \kappa l) + V^{S}(\kappa l, \kappa l) - K_\kappa]\, w_{\kappa l} \; . \end{aligned} \tag{2.53}$$

The mass m_s of the electron shell is negligible compared to the ionic mass m_κ. Therefore, the left hand side of equation (2.53) is approximately zero:

$$m_s \ddot{w}_{\kappa l} \approx 0 \; . \tag{2.54}$$

This condition is a mathematical formulation of the *adiabatic approximation*: The electron shell instantaneously occupies the position of minimum energy. Thus, equation (2.53) can be used to eliminate the shell coordinates $w_{\kappa l}$ from the equation of motion for the cores, equation (2.52). Adding equations (2.52) and (2.53) and replacing the shell coordinates $w_{\kappa l}$ by the *relative* displacement vectors $\bar{w}_{\kappa l}$ one obtains:

$$
\begin{aligned}
m_\kappa \ddot{u}_{\kappa l} = Z_\kappa \sum_{\kappa' l'} \sum V^C(\kappa l, \kappa' l') [Z_{\kappa'} u_{\kappa' l'} + Y_{\kappa'} \bar{w}_{\kappa' l'}] \; + \\
+ \sum_{\kappa' l'} \sum [V^{SR}(\kappa l, \kappa' l') + V^T(\kappa l, \kappa' l') + V^{T'}(\kappa l, \kappa' l') + V^S(\kappa l, \kappa' l')] \, u_{\kappa' l'} \; + \\
+ \sum_{\kappa' l'} \sum [V^T(\kappa l, \kappa' l') + V^S(\kappa l, \kappa' l')] \, \bar{w}_{\kappa' l'} \; + \\
+ [V^{T'}(\kappa l, \kappa l) - V^T(\kappa l, \kappa l)] \, \bar{w}_{\kappa l} \, .
\end{aligned}
\tag{2.55}
$$

Equation (2.53) is transformed into:

$$
\begin{aligned}
0 = Y_\kappa \sum_{\kappa' l'} \sum V^C(\kappa l, \kappa' l') [Z_{\kappa'} u_{\kappa' l'} + Y_{\kappa'} \bar{w}_{\kappa' l'}] \; + \\
+ \sum_{\kappa' l'} \sum [V^{T'}(\kappa l, \kappa' l') + V^S(\kappa l, \kappa' l')] \, u_{\kappa' l'} \; + \\
+ \sum_{\kappa' l'} \sum V^S(\kappa l, \kappa' l') \bar{w}_{\kappa' l'} \; + \; V^{T'}(\kappa l, \kappa l) \bar{w}_{\kappa l} - K_\kappa \bar{w}_{\kappa l} \, .
\end{aligned}
\tag{2.56}
$$

The term

$$
- \sum_{\kappa' l'} \sum V^C(\kappa l, \kappa' l') [Z_{\kappa'} u_{\kappa' l'} + Y_{\kappa'} \bar{w}_{\kappa' l'}]
$$

is the dynamical part of the effective electrical field at the equilibrium position of atom (κl).

Remembering the procedure of section 2.1, the equations of motion are solved by plane waves for $\mathbf{u}$ as well as for $\bar{\mathbf{w}}$. According to equations (2.8) and (2.15) one obtains the eigenvectors $\mathbf{e}_u$ and $\mathbf{e}_w$ for the motion of the cores and of the shells, respectively, and the last two equations are transformed into [3]:

$$
\begin{aligned}
\omega^2 \, \mathbf{e}_u = [\mathbf{M}(\mathbf{ZCZ} + \mathbf{F}^{SR} + \mathbf{F}^T + \mathbf{F}^{T'} + \mathbf{F}^S)\mathbf{M}] \; \mathbf{e}_u \; + \\
+ [\mathbf{M}(\mathbf{ZCY} + \mathbf{F}^T + \mathbf{F}^S + \mathbf{F}_o^{T'} - \mathbf{F}_o^T)\mathbf{M}] \; \mathbf{e}_w
\end{aligned}
\tag{2.57}
$$

and

$$
0 = [(\mathbf{YCZ} + \mathbf{F}^{T'} + \mathbf{F}^S)\mathbf{M}] \; \mathbf{e}_u \; + \; [(\mathbf{YCY} + \mathbf{F}^S + \mathbf{F}_o^{T'} - \mathbf{K})\mathbf{M}] \; \mathbf{e}_w \, . \tag{2.58}
$$

$\mathbf{M}$ being the mass tensor and $\mathbf{C}$ the matrix of Coulomb coefficients as defined by equations (2.20) and (2.41). $\mathbf{F}^{SR}$, $\mathbf{F}^T$, $\mathbf{F}^{T'}$ and $\mathbf{F}^S$ are the Fourier transforms of V^{SR}, V^T, $V^{T'}$ and V^S, respectively. $\mathbf{Y}$ and $\mathbf{K}$ are the diagonal matrices of the shell charges and the intraatomic shell-core force constants. $\mathbf{F}_o^T$ and $\mathbf{F}_o^{T'}$ contain the self-terms of the shell-core and the core-shell interactions. Both matrices have a block-diagonal form and the (3×3) submatrices along the diagonal are:

$$
\mathbf{F}_o^T(\kappa\kappa) = V^T(\kappa l, \kappa l) \tag{2.59}
$$

and

$$
\mathbf{F}_o^{T'}(\kappa\kappa) = V^{T'}(\kappa l, \kappa l) \, . \tag{2.60}
$$

It should be noticed that in contrast to all other matrices appearing in the equations (2.57) and (2.58), $\mathbf{F}^T$ and $\mathbf{F}^{T'}$ in general are *not* hermitian. This is due to the fact that the interaction between core (κl) and shell$(\kappa' l')$ is not necessarily the same as the interaction between core$(\kappa' l')$ and shell(κl). The hermitian conjugate matrix of $\mathbf{F}^{T'}$ is given by:

$$
(\mathbf{F}^{T'})^+ = \mathbf{F}^T + \mathbf{F}_o^{T'} - \mathbf{F}_o^T \, . \tag{2.61}
$$

Inspection of equations (2.57) and (2.58) yields that the *effective* short range contributions to the core-core, the shell-core, the core-shell and the shell-shell interactions are determined by the combinations

$$
\mathbf{F}^{CC} = \mathbf{F}^{SR} + \mathbf{F}^T + \mathbf{F}^{T'} + \mathbf{F}^S \, , \tag{2.62}
$$

$$
\mathbf{F}^{SC} = \mathbf{F}^{T'} + \mathbf{F}^S \, , \tag{2.63}
$$

$$
\mathbf{F}^{CS} = \mathbf{F}^T + \mathbf{F}^S + \mathbf{F}_o^{T'} - \mathbf{F}_o^T = (\mathbf{F}^{SC})^+ \tag{2.64}
$$

and

---

[3] For simplicity, the arguments qj labelling the different phonon states are omitted.

$$\mathbf{F}^{SS} = \mathbf{F}^{S} + \mathbf{F}_{o}^{T'} - \mathbf{K} \ , \tag{2.65}$$

respectively. Combining the two equations (2.57) and (2.58), $\mathbf{e}_w$ can be eliminated and one finally obtains the eigenvector equation for the motion of the ionic cores:

$$\omega^2 \mathbf{e}_u = \mathbf{M}\,[\mathbf{F}^{CC} + \mathbf{ZCZ} - (\mathbf{F}^{SC} + \mathbf{YCZ})^{+}(\mathbf{F}^{SS} + \mathbf{YCY})^{-1}(\mathbf{F}^{SC} + \mathbf{YCZ})]\,\mathbf{M}\,\mathbf{e}_u \ . \tag{2.66}$$

Thus, by comparison with equation (2.16), the total Dynamical Matrix turns out to be:

$$\mathbf{D} = \mathbf{M}[\mathbf{ZCZ} + \mathbf{F}^{CC} - (\mathbf{YCZ} + \mathbf{F}^{SC})^{+}(\mathbf{YCY} + \mathbf{F}^{SS})^{-1}(\mathbf{YCZ} + \mathbf{F}^{SC})]\mathbf{M} \ . \tag{2.67}$$

$^{+}$ denotes the hermitian conjugate matrix.

From equation (2.67) it can be seen that the shell model requires a special treatment: The polarization term, *i.e.* the third term on the right hand side of equation (2.67) has the form of a hermitian transformation in the 3N-dimensional space. Thus, all $(3N \times 3N)$ matrices appearing in equation (2.67) must be set up as a whole before the total Fourier transformed force constant matrix can be completed. It is not possible to calculate the (3×3) submatrices $\mathbf{D}(\kappa\kappa' \mid \mathbf{q})$ individually.

2.6 *Constraints for the Elements of the Dynamical Matrix*

The number of model parameters may become rather large if a complex structure or a complex interaction set-up is considered. There are, however, constraints for the force constant matrix and, hence, for the model parameters. These constraints arise from:

- the condition of translational invariance
- the condition of rotational invariance
- the condition of zero strain
- symmetry transformations.

2.6.1 Translational Invariance

A rigid translation of the crystal as a whole does not affect the interatomic potentials. As a consequence, there cannot be any force on any atom. In terms of the force constants this condition reads:

$$\sum_{\kappa' l'}\sum V(\kappa l, \kappa' l') = 0 \qquad \forall \quad (\kappa l) \ . \tag{2.68}$$

Usually, this condition is used to determine the self term $V(\kappa l, \kappa l)$, as pointed out in section 2.1.

2.6.2 Rotational Invariance

Similarly, a rigid rotation of the crystal as a whole does not affect the interatomic potential. Formally, the force in the direction α acting on the atom (κl) as a result of a rigid rotation around the x-, y- and z-axes can be written as:

$$f_{\alpha}^{x}(\kappa l) = \sum_{\kappa' l'}\sum [V_{\alpha y}(\kappa l, \kappa' l') r_z^{o}(\kappa' l') - V_{\alpha z}(\kappa l, \kappa' l') r_y^{o}(\kappa' l')] \tag{2.69}$$

$$f_{\alpha}^{y}(\kappa l) = \sum_{\kappa' l'}\sum [V_{\alpha z}(\kappa l, \kappa' l') r_x^{o}(\kappa' l') - V_{\alpha x}(\kappa l, \kappa' l') r_z^{o}(\kappa' l')] \tag{2.70}$$

$$f_{\alpha}^{z}(\kappa l) = \sum_{\kappa' l'}\sum [V_{\alpha x}(\kappa l, \kappa' l') r_y^{o}(\kappa' l') - V_{\alpha y}(\kappa l, \kappa' l') r_x^{o}(\kappa' l')] \ . \tag{2.71}$$

The condition of rotational invariance requires that all of these forces vanish.

In order to test a particular model the sums in equations (2.69)-(2.71) must be calculated numerically what may be difficult for long-range interactions. The invariance conditions can, however, be expressed by the Dynamical Matrix at small phonon wavevectors: Remembering its definition,

equation (2.13), $\mathbf{D}(\kappa\kappa'|\mathbf{q})$ may be expanded in a Taylor series of $\mathbf{q}$. Retaining the first-order terms one obtains:

$$\frac{1}{\sqrt{m_\kappa m_{\kappa'}}} e^{i\mathbf{q}(\mathbf{r}^\circ_{\kappa'} - \mathbf{r}^\circ_\kappa)} \mathbf{D}(\kappa\kappa'|\mathbf{q}) \simeq \sum_{l'} V(\kappa l, \kappa' l') + i\,\mathbf{q} \sum_{l'} (\mathbf{r}^\circ_{\kappa' l'} - \mathbf{r}^\circ_{\kappa l}) V(\kappa l, \kappa' l') \,. \tag{2.72}$$

Denoting

$$\mathbf{D}'(\kappa\kappa'|\mathbf{q}) = \frac{1}{\sqrt{m_\kappa m_{\kappa'}}} e^{i\mathbf{q}(\mathbf{r}^\circ_{\kappa'} - \mathbf{r}^\circ_\kappa)} \mathbf{D}(\kappa\kappa'|\mathbf{q}) \tag{2.73}$$

and

$$\begin{aligned} \delta\mathbf{q}_x &= (\delta q \;\; 0 \;\; 0) \\ \delta\mathbf{q}_y &= (0 \;\; \delta q \;\; 0) \\ \delta\mathbf{q}_z &= (0 \;\; 0 \;\; \delta q)\,, \end{aligned} \tag{2.74}$$

the following equation is obtained for small δq:

$$\mathbf{D}'(\kappa\kappa'|\delta\mathbf{q}_\alpha) = \sum_{l'} V(\kappa l, \kappa' l') + i\,\delta q \sum_{l'} V(\kappa l, \kappa' l')(\mathbf{r}^\circ_{\kappa' l'} - \mathbf{r}^\circ_{\kappa l})_\alpha \,. \tag{2.75}$$

By comparison with equations (2.69)-(2.71), the conditions of rotational invariance can now be expressed as:

$$f^x_\alpha(\kappa l) = \frac{1}{i\delta q} \sum_{\kappa'} [D'_{\alpha y}(\kappa\kappa'|\delta\mathbf{q}_z) - D'_{\alpha z}(\kappa\kappa'|\delta\mathbf{q}_y)] = 0 \tag{2.76}$$

$$f^y_\alpha(\kappa l) = \frac{1}{i\delta q} \sum_{\kappa'} [D'_{\alpha z}(\kappa\kappa'|\delta\mathbf{q}_x) - D'_{\alpha x}(\kappa\kappa'|\delta\mathbf{q}_z)] = 0 \tag{2.77}$$

$$f^z_\alpha(\kappa l) = \frac{1}{i\delta q} \sum_{\kappa'} [D'_{\alpha x}(\kappa\kappa'|\delta\mathbf{q}_y) - D'_{\alpha y}(\kappa\kappa'|\delta\mathbf{q}_x)] = 0 \,. \tag{2.78}$$

These sums can readily be evaluated, thus providing a test of rotational invariance.

For a system with central forces the matrix V can be represented by longitudinal and transverse force constants, equation (2.24). It can easily be shown that in this case the forces $f^\alpha_\alpha(\kappa l)$ vanish identically and $f^\alpha_\beta(\kappa l)$ is just the force in the direction $\alpha \times \beta$ acting on atom (κl) if all atoms occupy their equilibrium positions. Thus, the condition of rotational invariance is equivalent to the postulate that we are dealing with an equilibrium crystal structure.

2.6.3 Condition of Zero Strain

A crystal in its equilibrium state must not have internal strains. The comparison of the microscopic dynamics in the small $\mathbf{q}$ regime with the macroscopic description of elasticity leads to the following condition for zero strain:

$$\begin{aligned} G_{\alpha\beta\gamma\delta} = \sum_\kappa \sum_l \sum_{\kappa'} \sum_{l'} [&V_{\alpha\beta}(\kappa l, \kappa' l')(\mathbf{r}^\circ_{\kappa l} - \mathbf{r}^\circ_{\kappa' l'})_\gamma (\mathbf{r}^\circ_{\kappa l} - \mathbf{r}^\circ_{\kappa' l'})_\delta - \\ &- V_{\gamma\delta}(\kappa l, \kappa' l')(\mathbf{r}^\circ_{\kappa l} - \mathbf{r}^\circ_{\kappa' l'})_\alpha (\mathbf{r}^\circ_{\kappa l} - \mathbf{r}^\circ_{\kappa' l'})_\beta] \\ = 0 \,. \end{aligned} \tag{2.79}$$

This equation can be expressed in terms of the Dynamical Matrix at small $\mathbf{q}$ in analogy to the treatment in the preceeding section. Here, however, the second-order terms in the expansion according to equation (2.72) are involved:

$$\begin{aligned} G_{\alpha\beta\gamma\delta} = -\frac{1}{\delta q^2} \sum_\kappa \sum_{\kappa'} [&D'_{\alpha\beta}(\kappa\kappa'|\delta\mathbf{q}_\gamma + \delta\mathbf{q}_\delta) - D'_{\alpha\beta}(\kappa\kappa'|\delta\mathbf{q}_\gamma) - D'_{\alpha\beta}(\kappa\kappa'|\delta\mathbf{q}_\delta) - \\ &- D'_{\gamma\delta}(\kappa\kappa'|\delta\mathbf{q}_\alpha + \delta\mathbf{q}_\beta) + D'_{\gamma\delta}(\kappa\kappa'|\delta\mathbf{q}_\alpha) + D'_{\gamma\delta}(\kappa\kappa'|\delta\mathbf{q}_\beta)] \\ = 0 \,. \end{aligned} \tag{2.80}$$

The condition of zero strain, however, is not used very frequently for lattice-dynamical calculations.

2.6.4 Constraints Due to Symmetry

Obviously, symmetry operations which transform the crystal into itself provide further constraints to the elements of the force constant matrix and of the Dynamical Matrix. Suppose, there is a symmetry operation $(S|v)$[4] which sends the atom (κl) into the atom (λm) and simultaneously the atom $(\kappa' l')$ into $(\lambda' m')$. Then the elements $V(\kappa l, \kappa' l')$ and $V(\lambda m, \lambda' m')$ are no longer independent but can be calculated from one another. By consideration of the whole symmetry group the number of independent interactions can be obtained. The list of these interactions can be used as a guide for a proper model set-up.

For those symmetry operations $(S|v)$ which leave the phonon wavevector quasi-invariant:

$$S\,q = q + g \tag{2.81}$$

(g being a reciprocal lattice vector) the transformation of the Dynamical Matrix is given by:

$$D(\lambda\lambda'|q) = S\,D(\kappa\kappa'|q)\,e^{iq(r^0_\lambda - r^0_{\lambda'} - S(r^0_\kappa - r^0_{\kappa'}))}. \tag{2.82}$$

2.7 Amplitudes of Lattice Vibrations

According to equation (2.10) the displacement of a particular atom is given as a sum over the different phonon states (qj). In order to calculate phonon intensities as measured in neutron scattering experiments the amplitude of each lattice vibration (qj) at a given temperature has to be known. Especially for the investigation of lattice vibrations with high frequencies or at low temperatures, however, the quantum mechanical description is more adequate. The amplitude of a lattice mode is then obtained from the occupation probability of a phonon state.

In terms of the normal coordinates Q_{qj}, the Hamiltonian of the crystal system is given by equation (2.12) as a sum over the distinct and independent phonon states. Thus, each phonon state (qj) can be considered separately as a one-dimensional harmonic oscillator with respect to the normal coordinate Q_{qj}:

$$H_{qj} = \frac{1}{2N}[|\dot{Q}_{qj}|^2 + \omega^2_{qj}|Q_{qj}|^2]. \tag{2.83}$$

In quantum mechanical terms Q_{qj} and $\dot{Q}_{qj}$ correspond to the canonical conjugate operators Q and P which, in turn, can be represented by the creation and annihilation operators a^+ and a:

$$Q = \sqrt{\frac{\hbar}{2\omega_{qj}}}\,(a^+_{qj} + a_{qj}) \tag{2.84}$$

$$P = i\sqrt{\frac{\hbar\,\omega_{qj}}{2}}\,(a^+_{qj} - a_{qj}). \tag{2.85}$$

(For a more detailed discussion see textbooks on quantum mechanics.) Inserting these operators in equation (2.83) one gets:

$$H_{qj} = \hbar\,\omega_{qj}\,(a^+_{qj}a_{qj} + \frac{1}{2}). \tag{2.86}$$

The expectation value of a^+a is just the number of phonons n_{qj} with the energy $\hbar\,\omega_{qj}$ excited at a given temperature. $\hbar\,\omega_{qj}/2$ is the zero point energy. Phonons obey Bose-statistics, therefore $< a^-a >$ can be calculated as:

$$n_{qj} = < a^- a > = \frac{1}{\exp(\frac{\hbar\,\omega_{qj}}{k_B T}) - 1}. \tag{2.87}$$

The displacement operator for particle (κl) is obtained from equations (2.10) and (2.11) by replacing the coefficients A_{qj} and A^*_{qj} by the operators a_{qj} and a^-_{qj}, resp.:

---

[4] In this notation S is the rotational matrix and v is a fractional translation defining the symmetry transformation.

$$u_{\kappa l} = \frac{1}{\sqrt{Nm_\kappa}} \sum_q \sum_j e(\kappa | qj)\, e^{iqr_l}\, [a_{qj} e^{-i\omega_{qj}t} + a^{+}_{-qj} e^{i\omega_{qj}t}] . \tag{2.88}$$

The mean square amplitude of particle (κl) corresponding to a single phonon state (qj) is given by:

$$< |u^2_{\kappa l}| > = (n_{qj} + \frac{1}{2}) \frac{\hbar}{Nm_\kappa \omega_{qj}} , \tag{2.89}$$

and in the classical limit:

$$\begin{aligned} n_{qj} &\rightarrow \frac{k_B T}{\hbar \omega_{qj}} \\ < |u^2_{\kappa l}| > &\rightarrow \frac{k_B T}{N m_\kappa \omega^2_{qj}} \end{aligned} \tag{2.90}$$

2.8 *Phonon Intensities in Neutron Scattering*

Inelastic neutron scattering is the unique experimental method for the determination of phonon dispersion curves. Phonon intensities vary, however, from one Brillouin zone to the other, depending on the particular eigenvector. Therefore, it is sometimes a rather hard task to detect special phonons experimentally. In this case, lattice-dynamical calculations may provide a guide for the optimization of experiments.

In neutron scattering experiments a monochromatized beam characterized by the wavevector $\mathbf{k}_i$ hits the sample and one asks for the number of neutrons leaving the sample with the wavevector $\mathbf{k}_f$. The scattering probability and, hence, the scattered intensity is essentially determined by the

momentum transfer[5]

$$\hbar \mathbf{Q} = \hbar (\mathbf{k}_i - \mathbf{k}_f) \tag{2.91}$$

and the

energy transfer

$$\hbar \omega = \frac{\hbar^2}{2m_n} (k_i^2 - k_f^2) , \tag{2.92}$$

(m_n being the neutron mass). Due to resolution and normalizing effects the intensity does, in fact, depend on the special choice of $\mathbf{k}_i$ and $\mathbf{k}_f$ but the response of the sample itself can be described in terms of Q and ω. $\hbar$ Q and $\hbar\omega$ are the momentum and the energy, resp., which are transferred *to* the sample during the scattering process and equations (2.91) and (2.92) are the laws of momentum and energy conservation. We will not give a review of the fundamentals of neutron scattering here. We only want to recall that phonons are collective excitations of the crystal lattice and, hence, it is the coherent part of the scattering which carries the information about the distinct phonon states. For details the reader is referred to the literature, *e.g.* [8].

The calculation of phonon intensities, of the so-called *dynamical structure factor*, starts from the following expression for the coherent scattering function S_{coh} which is proportional to the scattered intensity:

$$S_{coh}(\mathbf{Q}, \omega) = \frac{1}{N} \int \sum_\kappa \sum_l \sum_{\kappa'} \sum_{l'} b_\kappa b^*_{\kappa'} e^{-iQ(r^0_{\kappa l} - r^0_{\kappa' l'})} < e^{-iQ(u_{\kappa l}(t) - u_{\kappa' l'}(0))} > dt , \tag{2.93}$$

where b_κ and $b_{\kappa'}$ are the coherent scattering lengths of particles of type κ and κ', resp.. Using the results of section 2.7 for the atomic displacements **u** of a harmonic crystal and expanding the phase factor in equation (2.93) in powers of $\mathbf{u}_{\kappa l}(t) - \mathbf{u}_{\kappa' l'}(0)$, one obtains after some calculation for the *one-phonon scattering, i.e.* the first-order term in the displacements:

---

[5] Different from the convention followed in the other parts of this manual, here the capital bold printed letter Q denotes a vector rather than a matrix. The reason for this inconsistency is, that in the literature concerning neutron scattering the scattering vector is almost exclusively denoted by Q.

ERRATA

Unfortunately, after printing some mistakes concerning the signs in several equations have been detected. The reader is asked to replace the following formulae:

Equation (2.24) on page 6 should read:

$$V_{\alpha\beta}(\kappa l, \kappa' l') = -(L - T)\frac{r_\alpha r_\beta}{r^2} - T\,\delta_{\alpha\beta}\,. \tag{2.24}$$

Equation (2.52) on page 9 should read:

$$\begin{aligned} m_\kappa \ddot{u}_{\kappa l} = & -X_\kappa \sum_{\kappa' l'}\sum V^C(\kappa l, \kappa' l')\,[X_{\kappa'} u_{\kappa' l'} + Y_{\kappa'} w_{\kappa' l'}] - \\ & - \sum_{(\kappa' l') \neq (\kappa l)} [V^{SR}(\kappa l, \kappa' l') u_{\kappa' l'} + V^T(\kappa l, \kappa' l') w_{\kappa' l'}] + \\ & + K_\kappa w_{\kappa l} - [V^{SR}(\kappa l, \kappa l) + V^T(\kappa l, \kappa l) + K_\kappa]\, u_{\kappa l}\,. \end{aligned} \tag{2.52}$$

Equation (2.53) on page 9 should read:

$$\begin{aligned} m_s \ddot{w}_{\kappa l} = & -Y_\kappa \sum_{\kappa' l'}\sum V^C(\kappa l, \kappa' l')\,[X_{\kappa'} u_{\kappa' l'} + Y_{\kappa'} w_{\kappa' l'}] - \\ & - \sum_{(\kappa' l') \neq (\kappa l)} [V^{T'}(\kappa l, \kappa' l') u_{\kappa' l'} + V^S(\kappa l, \kappa' l') w_{\kappa' l'}] + \\ & + K_\kappa u_{\kappa l} - [V^{T'}(\kappa l, \kappa l) + V^S(\kappa l, \kappa l) + K_\kappa]\, w_{\kappa l}\,. \end{aligned} \tag{2.53}$$

Equation (2.55) on page 10 should read:

$$\begin{aligned} -m_\kappa \ddot{u}_{\kappa l} = & Z_\kappa \sum_{\kappa' l'}\sum V^C(\kappa l, \kappa' l')\,[Z_{\kappa'} u_{\kappa' l'} + Y_{\kappa'} \bar{w}_{\kappa' l'}] + \\ & + \sum_{\kappa' l'}\sum [V^{SR}(\kappa l, \kappa' l') + V^T(\kappa l, \kappa' l') + V^{T'}(\kappa l, \kappa' l') + V^S(\kappa l, \kappa' l')]\, u_{\kappa' l'} + \\ & + \sum_{\kappa' l'}\sum [V^T(\kappa l, \kappa' l') + V^S(\kappa l, \kappa' l')]\, \bar{w}_{\kappa' l'} + \\ & + [V^{T'}(\kappa l, \kappa l) - V^T(\kappa l, \kappa l)]\, \bar{w}_{\kappa l}\,. \end{aligned} \tag{2.55}$$

Equation (2.56) on page 10 should read:

$$\begin{aligned} 0 = & Y_\kappa \sum_{\kappa' l'}\sum V^C(\kappa l, \kappa' l')\,[Z_{\kappa'} u_{\kappa' l'} + Y_{\kappa'} \bar{w}_{\kappa' l'}] + \\ & + \sum_{\kappa' l'}\sum [V^{T'}(\kappa l, \kappa' l') + V^S(\kappa l, \kappa' l')]\, u_{\kappa' l'} + \\ & + \sum_{\kappa' l'}\sum V^S(\kappa l, \kappa' l') \bar{w}_{\kappa' l'} + V^{T'}(\kappa l, \kappa l) \bar{w}_{\kappa l} + K_\kappa \bar{w}_{\kappa l}\,. \end{aligned} \tag{2.56}$$

Line 10 on page 10 should read:

$$\sum_{\kappa' l'}\sum V^C(\kappa l, \kappa' l')[Z_{\kappa'} u_{\kappa' l'} + Y_{\kappa'} \bar{w}_{\kappa' l'}]\,.$$

Equation (2.58) on page 10 should read:

$$0 = [(\mathbf{YCZ} + \mathbf{F}^{T'} + \mathbf{F}^S)\mathbf{M}]\ \mathbf{e}_u + [(\mathbf{YCY} + \mathbf{F}^S + \mathbf{F}_o^{T'} + \mathbf{K})\mathbf{M}]\ \mathbf{e}_w\,. \tag{2.58}$$

Equation (2.65) on page 11 should read:

$$\mathbf{F}^{SS} = \mathbf{F}^S + \mathbf{F}_o^{T'} + \mathbf{K}\,. \tag{2.65}$$

In program **NN** an additional storage option is included: Please add the following line in the description of the input card 1 for program **NN** on page 25:

IDIR(3) = 0 (1) (no) storage of data.

$$S_{coh}^{(1)}(\mathbf{Q},\omega) = \frac{1}{N}\sum_{\mathbf{q}}\sum_{j} S_{coh}^{(\mathbf{qj})}(\mathbf{Q},\omega)\,, \tag{2.94}$$

$S_{coh}^{(\mathbf{qj})}$ being the partial scattering function due to the single phonon state (**qj**):

$$S_{coh}^{(\mathbf{qj})}(\mathbf{Q},\omega) = \frac{\hbar}{\omega_{\mathbf{qj}}}\Big|\sum_{\kappa}\frac{b_\kappa e^{-W_\kappa}}{\sqrt{m_\kappa}}\,\mathbf{Q}\,e(\kappa\,|\,\mathbf{qj})\Big|^2 \bullet \\ \bullet\{[n_{\mathbf{qj}}+1]\delta(\omega-\omega_{\mathbf{qj}}) + n_{\mathbf{qj}}\delta(\omega+\omega_{\mathbf{qj}})\}\sum_{\mathbf{g}}\delta_{\mathbf{Q},\,\mathbf{g}+\mathbf{q}}\,. \tag{2.95}$$

e^{-W_κ} is the Debye-Waller factor of particles of type κ. The δ-functions on the right hand side of equation (2.95) reflect the energy and momentum conservation since the phonon (**qj**) carries the energy $\hbar\omega_{\mathbf{qj}}$ and the momentum $\hbar\,\mathbf{q}$. In periodic structures, the wavevector of excitations is always defined modulo a reciprocal lattice vector **g**. Therefore, every phonon can in principle be measured in every Brillouin zone **g**. This is taken into account by the sum over **g** in equation (2.95). Furthermore, a phonon can be created or absorbed by a neutron corresponding to δ-peaks at positive or negative frequency. Obviously, the creation of a phonon is more likely than the absorption, since in the latter case the phonon must already be excited. The phonon intensity is thus larger at $+\,\omega_{\mathbf{qj}}$ than at $-\,\omega_{\mathbf{qj}}$. The asymmetry of the spectra is given by the condition of *Detailed Balance*:

$$\frac{I(\omega_{\mathbf{qj}})}{I(-\omega_{\mathbf{qj}})} = \frac{n_{\mathbf{qj}}+1}{n_{\mathbf{qj}}} = \exp\left(\frac{\hbar\,\omega_{\mathbf{qj}}}{k_B T}\right). \tag{2.96}$$

Phonons can, however, be observed only if their polarization vector **e(qj)** has a component in the direction of the momentum transfer. Mathematically, this is described by the dot-product **Qe** in equation (2.95). Thus, lattice-dynamical calculations which directly yield the frequencies and the polarization vectors can be used to predict phonon intensities which may be obtained in neutron scattering experiments.

2.9 *The Symmetry of Lattice Vibrations*

The Dynamical Matrix and its eigenvectors are functions of the atomic positions within the crystal and can thus be represented by symmetry-adapted functions. Since **D** is also a function of the phonon wavevector **q** the following discussion is restricted to symmetry operations which leave the wavevector invariant. These symmetry operations form the *group of the wave vector* G_q which is a subgroup of the total symmetry group G_o. The symmetry adapted functions or *symmetry coordinates* are the basis vectors for the various irreducible multiplier representations (IMR) of G_q. The eigenvectors of the Dynamical Matrix can be represented as a linear combination of the symmetry coordinates of one single representation. Thus, the eigenvectors are labelled according to their symmetry.

The transformation of the Dynamical Matrix under the operations of G_q is given by equation (2.82) and provides a 3N-dimensional (reducible) representation Γ_{3N} of G_q, the set of 3N cartesian coordinates generating the corresponding vector space. As a result from group theory, there is a finite number of irreducible multiplier representations γ_i of G_q and Γ_{3N} may be represented as the direct sum:

$$\Gamma_{3N} = \sum_{i} m_i\gamma_i\,, \tag{2.97}$$

m_i being the multiplicity of γ_i. Correspondingly, the 3N-dimensional vector space is decomposed into several subspaces of lower dimensions which are invariant under the operations of G_q. A basis of each of these subspaces can be constructed by projector techniques as described in [4]. With respect to these new symmetry coordinates which are linear combinations of the 3N cartesian coordinates, the Dynamical Matrix is block-diagonalized. The dimensions of the individual blocks are given by the multiplicity of the corresponding IMR.

Let $\mathbf{x}_i^j$ be a 3N-dimensional vector transforming according to the i-th IMR ($1 \ldots m_i$). If all the vectors $\mathbf{x}_i^j$ are pairwise orthonormal they form the set of symmetry coordinates:

$$\mathbf{X} = (\mathbf{x}_1^1 \ldots \mathbf{x}_1^{m_1}\mathbf{x}_2^1 \ldots) \tag{2.98}$$

The block-diagonalized Dynamical Matrix is given by the transformation:

$$\mathbf{D}^X = \mathbf{X}^{-1}\,\mathbf{D}\,\mathbf{X}\,. \tag{2.99}$$

Each block i of this matrix can now be diagonalized individually. All corresponding eigenvectors $\mathbf{e}_i^X$ belong to the same IMR. Thus, the different vibrational modes are automatically arranged according to their symmetry. The eigenvectors are retransformed to cartesian coordinates by:

$$\mathbf{e}_i = \mathbf{X}\,\mathbf{e}_i^X . \tag{2.100}$$

More detailed information about the group-theoretical analysis of lattice vibrations including time-reversal conditions etc. are given in the review article by *MARADUDIN* and *VOSKO* [4].

For the practical work with the program package UNISOFT, however, it is sufficient to know that there is a set of symmetry coordinates which provides the decomposition of the Dynamical Matrix and its eigenvectors according to different symmetries. These symmetry coordinates can be calculated simply on the basis of group theory for each crystal structure without any other assumption.

2.10 *Static Electrical Field and Gradients*

Within the framework of lattice dynamics based on Coulomb interactions the static electrical field **h** and the field gradient **H** at the position of any atom (κl) may be calculated. **h** is proportional to the gradient of the total electrostatic potential except the self potential and **H** is the matrix of second derivatives:

$$h_\alpha(\kappa l) = -\frac{1}{Z_\kappa}\sum_{\kappa' l'}\sum \frac{\partial V^c_{\kappa\kappa'}(r)}{\partial r_\alpha}\Big|_{r = r^o_{\kappa l} - r^o_{\kappa' l'}} \tag{2.101}$$

$$H_{\alpha\beta}(\kappa l) = -\frac{1}{Z_\kappa}\sum_{\kappa' l'}\sum \frac{\partial^2 V^c_{\kappa\kappa'}(r)}{\partial r_\alpha \partial r_\beta}\Big|_{r = r^o_{\kappa l} - r^o_{\kappa' l'}} . \tag{2.102}$$

Obviously, **H** is closely related to the matrix of Coulomb coefficients defined in section 2.3:

$$\mathbf{H}(\kappa l) = \sum_{\kappa'} Z_{\kappa'} C(\kappa\kappa' | \mathbf{q} \to 0) - \frac{Z_\kappa}{3\varepsilon_o}\sqrt{\frac{p}{\pi}}^3 \mathbf{I}, \tag{2.103}$$

(**I** being the unit matrix). Note that the sum on the right hand side of equation (2.103) does *not* depend on the direction from which $\mathbf{q} = 0$ is approached whereas the Coulomb coefficients itselves do (see footnote [2] on page 7). The second term is due to the self potential of the Gaussian charge distribution which is used for the evaluation of the Coulomb coefficients (compare section 2.3). **C** contains the self term and **H** does not.

The electrical field can be calculated by Ewald's method in analogy to equations (2.34)-(2.39):

$$h_\alpha(\kappa l) = \frac{i}{v\varepsilon_o}\sum_{\kappa'} Z_{\kappa'} \sum_{\mathbf{g}} \frac{g_\alpha}{|\mathbf{g}|^2} \exp\left[-\frac{g^2}{4p}\right] \exp\left[ig(r^o_\kappa - r^o_{\kappa'})\right] + \\ + \sum_{\kappa' l'}\sum \frac{1}{Z_{\kappa'}} \frac{\partial V^{overlap}_{\kappa\kappa'}(r)}{\partial r_\alpha}\Big|_{r = r^o_{\kappa l} - r^o_{\kappa' l'}} . \tag{2.104}$$

The last two equations allow to calculate electrostatic properties of crystals quite generally. Thus, lattice-dynamical methods can be applied not only to phonon investigations but also to other experimental techniques such as nuclear quadrupole resonance etc..

3.0 Structure of UNISOFT

The program package UNISOFT allows to perform a lattice-dynamical treatment of crystals with up to 20 atoms per primitive cell. There are no restrictions on crystal symmetry and structure and phonon wavevectors can be chosen arbitrarily. At present, UNISOFT consists of nine individual programs written in FORTRAN IV and running on the IBM 3033-U12 computer at the Nuclear Research Center Jülich. In particular, these programs deal with the following topics:

Program	*Topic*
GROUP	Group-theoretical analysis of the crystal structure
IND	Determination of independent interactions
NN	Neighbourhood analysis of each atom in the crystal
MODEL1	Model calculations
HIST	Histogram of dispersion curves
SF	Dynamical structure factors
PARDER	Partial derivatives of phonon frequencies
ROTINV	Test of rotational invariance
EFG	Electrical fields and their gradients.

The individual programs communicate with each other via four different disk-datasets:

COORD contains informations about the space group of the crystal and about the group of the wavevector for every **q** selected as well as the symmetry coordinates.

INDDAT contains the number of independent interactions and for each of these a representative pair of atoms.

XNN contains for each pair of atoms the vectors for up to the 10th nearest neighbours arranged in neighbouring shells (pair correlation vectors).

RESULT contains the results of model calculation including the matrix of Coulomb coefficients, eigenvectors and eigenvalues.

Figure 2 on page 18 displays the structure of UNISOFT and the communication between the different programs. Obviously, for a given crystal structure the programs **IND** and **NN** need to be run only once. **GROUP**, however, has to be invoked whenever a new set of phonon wavevectors is considered since the symmetry coordinates depend on **q** and are needed in subsequent programs.

GROUP has been developed by *WARREN* and *WORLTON* [9]. It has been slightly modified in order to be compatible with the communication features of UNISOFT. All the other programs have a rigorous modular structure. They are tailored on the basis of rather small subroutines each of which deals with a very specific task. Therefore, some of the subroutines can be used in different programs. A complete list of all subroutines used within UNISOFT is given in appendix C. The modular structure of UNISOFT offers the possibility to extend this program package rather easily. Thus, in existing programs new features may be implemented such as new interaction potentials in **MODEL1**. On the other hand, separate new programs may be added which make use of previous results and which may contain one or more of the existing general subroutines. Examples for possible extensions are briefly discussed in section 6.

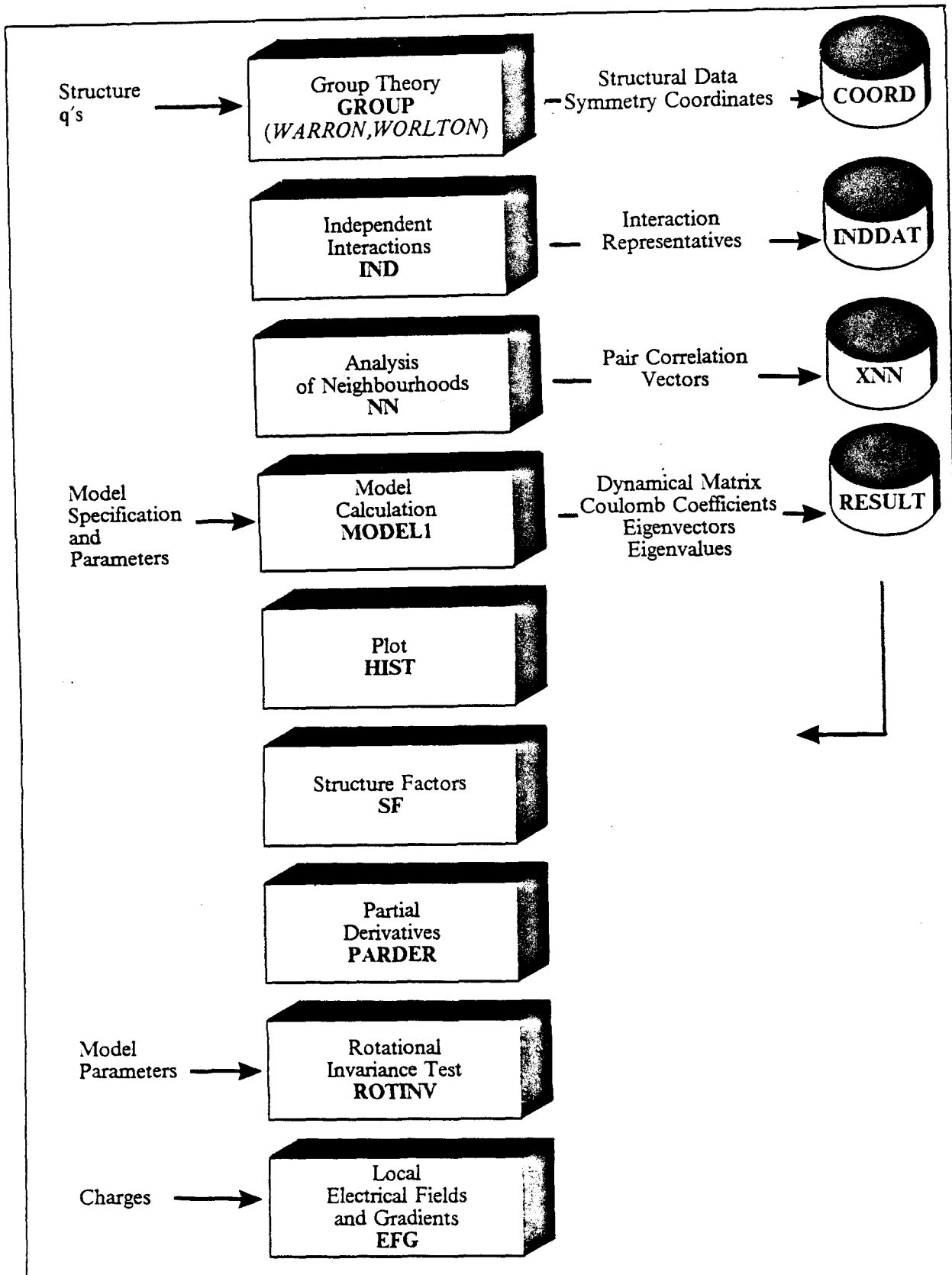

Figure 2. Structure of the program package UNISOFT

In the following chapter, a detailed description of the purpose of each individual program is given along with the instructions for use.

4.0 Detailed Description of the Individual Programs

4.1 GROUP

4.1.1 General Purpose

The program **GROUP** performes a group-theoretical analysis of a given crystal structure. It is described in detail by *WARREN* and *WORLTON* [9]. Here, we only want to give a short review of the facilities of this program which are important for subsequent lattice-dynamical calculations. **GROUP** has been slightly modified compared to the original version of *WARREN* and *WORLTON* in order to meet the requirements for the communication with the other programs of UNISOFT.

The theoretical foundation of **GROUP** is the review article of *MARADUDIN* and *VOSKO* [4] where the symmetry constraints for the lattice vibrations are investigated in a general way.

Given the basis vectors of the primitive cell and the position vectors of *all* atoms within this cell, the program determines the symmetry operations transforming the infinite crystal into itself, *i.e.* the space group of the lattice. If desired, the atom transformation table and the multiplication table for the symmetry operations are printed.

The set of phonon wavevectors **q** for which lattice-dynamical calculations are to be performed is selected in **GROUP**. For each value of **q** the point group G_q of the rotational parts of symmetry operations which leave **q** invariant (modulo a reciprocal lattice vector) is determined along with the set of irreducible multiplier representations (IMR) of G_q.

For N atoms per primitive cell the vector space of the 3N cartesian coordinates provides a 3N-dimensional representation Γ_{3N} of G_q according to equation (2.82) on page 13. This representation may be written as a direct sum of several of the irreducible representations γ_i:

$$\Gamma_{3N} = \sum_i m_i \gamma_i \,. \tag{4.1}$$

The multiplicity m_i of the i-th IMR in this decomposition is given by the characters χ of Γ and χ_i of γ_i:

$$m_i = \frac{1}{G} \sum_i \chi_i^*(g)\, \chi(g) \,, \tag{4.2}$$

where G is the order of G_q and the sum runs over all elements g of G_q. Basis vectors for the corresponding invariant subspaces are found by projector techniques as described in [4]. These so-called *Symmetry Coordinates* are used for the block diagonalization of the Dynamical Matrix as discussed in section 2.9. By diagonalizing the individual blocks of the Dynamical Matrix separately, the eigenvectors will be arranged automatically according to their symmetry.

The form of the symmetry-reduced Dynamical Matrix can be obtained without a specific lattice-dynamical model simply from group theory: The number of independent elements of the Dynamical Matrix is given by:

$$n = \frac{1}{2} \sum_i m_i(m_i + 1) \tag{4.3}$$

as a direct consequence of the irreducible decomposition. This number might, however, be further reduced if there is a symmetry operation which transformes **q** into -**q** since $\mathbf{D}(-\mathbf{q}) = \mathbf{D}^*(\mathbf{q})$.

Numerically, independent elements can be found in the following way: Starting from a random hermitian matrix all the symmetry elements of G_q are applied according to equation (2.82). Comparing the resultant and the original matrices, those elements which have to be identical are detected as well as those which have to be zero. Thus, representing different elements by different alphabetical symbols and zero elements by a dot (.), a symbolic symmetry reduced Dynamical Matrix is obtained. This reduction, however, may be incomplete since the computer does not realize if two elements are linked by a well defined factor such as $1/2$, 2, -1, $\sqrt{3/2}$ etc.. Nevertheless, the symbolic form of the (partially) reduced Dynamical Matrix which is calculated in **GROUP** may provide some feeling for symmetry constraints since this matrix is defined with respect to the cartesian particle coordinates. Using the symmetry coordinates, the symbolic matrix is transformed into a block diagonalized form. This representation, however, may be less illustrative since it is defined in the vector space of the symmetry coordinates.

For the Γ-point (zero wavevector) G_q obviously is the whole point group of the lattice. The selection rules for Raman and infrared active modes are determined by symmetry and, hence, can be detected simply by the application of group theory.

Note that in systems with Coulomb interactions lattice-dynamical calculations cannot be performed exactly for $\mathbf{q} = 0$ without taking into account retardation effects (c.f. footnote [2] on page 7). In these cases, Γ-point modes are calculated by considering very small but non-zero wavevectors $\delta\mathbf{q}$. The group-theoretical treatment, however, should be based on the whole point group of the lattice even if, striktly speaking, $\delta\mathbf{q}$ is of lower symmetry. Consequently, all wavevectors with moduli smaller than 0.001Å^{-1} are interpreted within **GROUP** as being zero.

4.1.2 The Position of GROUP within the Framework of UNISOFT

In a lattice-dynamical treatment of a crystal structure **GROUP** has to be invoked as the first program. Since the symmetry coordinates depend on the phonon wavevector $\mathbf{q}$ the program **GROUP** also has to be run whenever a new set of $\mathbf{q}$-values is selected.

The structural parameters including the position vectors of all atoms per primitive cell and the symmetry operations are written on the disk dataset **COORD** (logical unit 1). For each value of the phonon wavevector the irreducible representations and the corresponding calculated symmetry coordinates are saved on **COORD** as well and can be used by other programs.

4.1.3 Input

Card 1 **Comment** [18A4]
This comment is used as a header for the printed output.

Card 2 **NA, IPM, IDC, NCC, NX** [5I5]
NA = Number of atoms per primitive cell (≤ 20)
IPM = 1 if printing of multiplication table of the space group is desired
IDC = 0(1) if the D-(C)-definition according to *MARADUDIN* and *VOSKO* of the Dynamical Matrix is to be used (see footnote [1] on page 4)
In order to be compatible with other programs of UNISOFT use the D-definition, IDC = 0, always!
NCC = Number of comment double-cards given below
NX = Number of additional atoms (outside the primitive cell) the positions of which will be given to make sure that the space group of the crystal will be determined correctly. In most cases NX can be set to zero. Only if the proper space group is not found it may be necessary to use NX > 0.

Card 3 **(NAME(I), I = 1,NA)** [18A4]
NAME(I) = symbolic name for atom I (in general the chemical symbol) which is used to provide a more illustrative output

Card 4 **Comment** [33A4]
NCC (double cards) of format [33A4] providing more detailed information about the structure under consideration

Card 5 **((A(I,J), I = 1,3), J = 1,3)** [9F8.5]
A(I,J) = I-th cartesian coordinate of the J-th basis vector of the primitive cell in the direct space in Å

For each of the NA + NX atoms one card of the following type must be given:

Card 6 **TY, (X(I), I = 1,3), JM** [I5,3F10.5,I5]
TY = type number of the atom
This parameter is used to distinguish between different kinds of atoms. Symmetrical equivalent atoms obviously are of the same type. This is, however, not necessarily the case for all chemically identical atoms: Rather, atoms which are expected to have different interaction parameters have to be of different types.
X(I) = I-th cartesian coordinate of the position vector in Å
JM = 1(0) if the unit is a molecule (atom)
Since in the present version, UNISOFT deals with atomic structures only, use JM = 0 always!

Card 7 (QS(I), I = 1,3) [3F10.5]
QS(I) = I-th cartesian coordinate in $Å^{-1}$ of a vector QS used for scaling wavevector input.
If QS(I) = 0 wavevectors are scaled according to the intersection of the cartesian axes with the Brillouin zone boundary (not exactly in the case of more complicated structures - check by yourself!).

Card 8 **NIR, IT** [2I5]
Control card:
NIR = 0 program stop
= 1 program continue
= -1 program restart
IT = 0,1,...8 control parameter for output list
A larger value of IT corresponds to more printed informations. Please, check by yourself the effect of IT.

Card 9 **Comment** [18A4]
For each value of the phonon wavevector a separate comment can be given.

Card 10 (Q(I), I = 1,3) [3F10.5]
Q(I) = I-th cartesian coordinate of the wavevector in units of QS(I) or in units of the zone boundary (see card 7)

You may continue the input by giving the cards 8.- 10. for other values of Q. The program stops reading further input cards if it detects a card of type 8 with NIT = 0.

4.1.4 Output

The extent of the printed output is determined by the parameter IT (card 8). For larger values of IT even intermediate results during the determination of irreducible representations are printed. The user is recommended to try the different possibilities of output control by himself.

If **GROUP** is run for the first time for a given structure the results of the space group determination should carefully be examined. In some cases it might be necessary to give coordinates of additional atoms outside the first primitive cell in order to make sure that the program will find the correct space group.

An example is given in appendix A.1, page 53.

4.2 *IND*

The program **IND** determines the number of different types of atoms and the independent interactions in a crystal which has been defined by the input of the program **GROUP**. As pointed out in section 2.6.4 a list of independent, *i.e.* symmetrical inequivalent, interactions as produced by **IND** may serve as a guide for a proper set-up of a lattice-dynamical model. This is especially useful for more complicated structures since a multiple (and perhaps inconsistent) definition of the same interaction can easily be avoided.

IND has to be run only once for a given structure. It does not need any user input but reads the structural information from the disk-dataset **COORD** (logical unit 1). Thus, **GROUP** has to be run first. The output is printed as well as stored on the file **INDDAT** (logical unit 3) for further use by subsequent programs. An example is given in appendix A.2, page 60.

4.3 NN

4.3.1 General Purpose

The program **NN** analyzes the neighbourhood of each atom in the primitive cell. Since the calculation of a Dynamical Matrix requires the evaluation of a lattice sum corresponding to equations (2.18) or (2.38) it is convenient to arrange the neighbours of a given atom in spherical shells. The lattice sums are rapidly convergent and only near neighbours need to be considered. For each pair of atoms κ and κ' up to 10 neighbouring shells are examined: *i.e.*, particles κ' in different primitive cells l' are arranged according to their distance with respect to atom κ in cell 0. All atoms $\kappa' l'$ which exhibit the same or nearly the same distance are said to belong to the same shell (see Figure 3 on page 25). Obviously, the interactions between κ and all atoms κ' within a shell are identical at least for central force models.

The program **NN** lists the difference vectors $\mathbf{r}_{\kappa 0} - \mathbf{r}_{\kappa' l'}$ for all atoms within these shells. In parallel, the data are stored on the disk-dataset **XNN**. Subsequent programs like **MODEL1**, **PARDER** or **EFG** make use of the ordered arrangement of the atoms: The lattice sum of equation (2.18) is replaced by the sum over all particles of the first neighbouring shells. Furthermore, for complicated structures also the set-up of a lattice-dynamical model itself is simplified using the results of **NN**: Since **NN** essentially determines the pair-correlation one can immediately select the most important interactions which have to be specified in the model. In slightly distorted structures, *e.g.*, often two or more shells are rather close to one another. Thus, the neglect of interactions with atoms of one of these shells can lead to unreasonable results.

The number of atoms κ' which are located at a given distance from an atom κ defines the partial pair-correlation function. The program **NN** offers the possibility to display this correlation function as a histogram plot. Remembering that several atoms within the primitive cell might belong to the same type, it can be even more illustrative to plot the *type-dependent correlation function*, *i.e.* the number of particles of the same type located at a given distance.

The number of shells to be examined for each pair of atoms κ and κ' can be chosen between 1 and 10. The thickness of the shells is given in Å. Note, however, that both parameters have to be selected in a way to guarantee that the number of atoms per shell does not exceed 30!

4.3.2 The Position of NN within the Framework of UNISOFT

NN needs to be run only once for a given structure. The structural information is read from the file **COORD** (logical unit 1). If a plot of the type-dependent pair-correlation function is required the information about the different types of atoms is read from **INDDAT** (logical unit 2). Thus, **GROUP** and **IND** have to be run first. The distance vectors of all atoms in the shells examined are written on the disk-dataset **XNN** (logical unit 3). These data provide the input for other programs like **MODEL1**, **PARDER** or **EFG**.

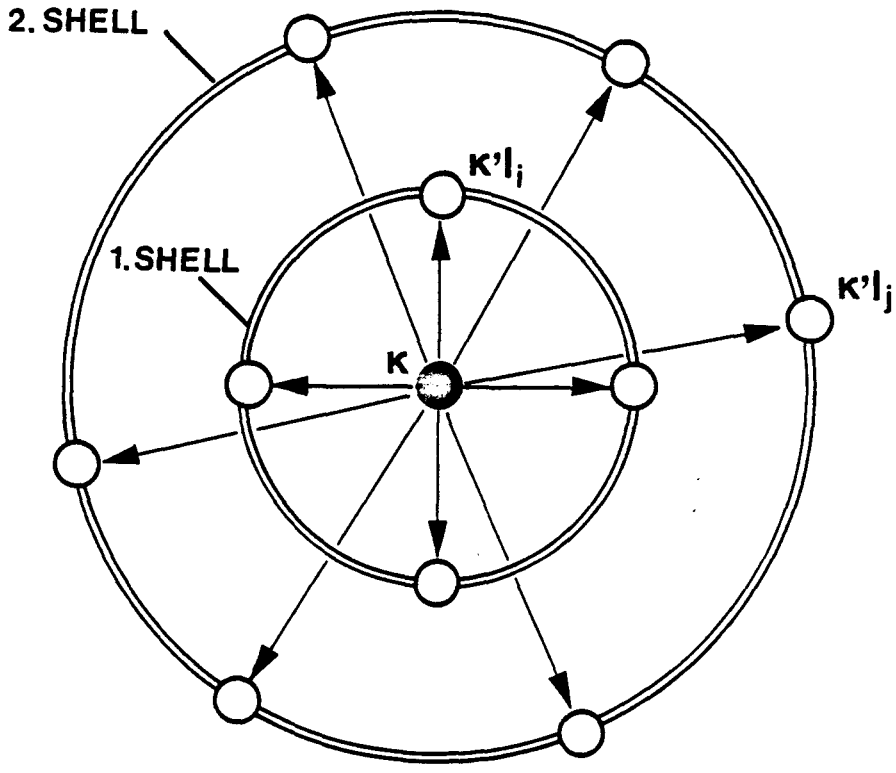

Figure 3. **The concept of neighbouring shells:**
Atom K in cell 0 (●) surrounded by atoms K′ in different cells l_i, l_j, ...(o).

4.3.3 Input

Card 1 **(IDIR(I), I = 1,3)** [3I5]
Output Control:
IDIR(1) = 1 (0) with (without) printout
IDIR(2) = 0 no histogram of pair correlation function (pcf)
IDIR(2) = 1 histogram of atom specific pcf
IDIR(2) = 2 histogram of type specific pcf
(may be useful if several atoms within the primitive cell belong to the same type)

Card 2 **NNS** [I5]
NNS = maximum number of shells to be examined.
NNS ≤ 10 and NNS has to be chosen in a way to guarantee that the number of atoms per shell is not larger than 30.

Card 3 **DELTA, DMAX** [2F10.6]
DELTA = thickness of a shell in Å
DMAX = maximum shell radius in Å for histogram-plot

4.3.4 Output

The output may become rather voluminous especially for more complicated structures with many particles per unit cell. An excerpt of an example is given in appendix A.3, page 61.

4.4 MODEL1

4.4.1 General Purpose

The program **MODEL1** calculates phonon frequencies and eigenvectors for the particular structure analyzed in the preceeding programs **GROUP**, **IND** and **NN**. It can thus be regarded as the heart of UNISOFT wheras the other programs are auxiliary routines. The phonon wavevectors are chosen arbitrarily in **GROUP** since the group-theoretical treatment, *i.e.* the calculation of symmetry coordinates, depends on $\mathbf{q}$ (see section 2.9).

A lattice-dynamical model set-up requires the specification of all (pair-) interactions within a particular structure. In most cases, interactions (other than Coulomb interactions) will be restricted to near neighbours. Sometimes, force constants may be calculated from interatomic potentials, but if a reliable potential does not exist, *e.g.* for covalent bonds, the force constants itselves are considered as model parameters (Born-von Karman model). In the latter case, the number of model parameters may become rather large if more neighbouring shells are taken into account. The essential feature of **MODEL1** is the fact that the interaction between each pair of atoms can be modelled individually by selecting one or more of the following interaction types which are implemented presently:

1. Born-von Karman model (longitudinal and transverse springs)
2. Born-Mayer potential
3. Lennard-Jones potential
4. van der Waals potential
5. Coulomb potential
6. shell model.

This list may be extended rather easily if necessary. The combination of different interactions for different pairs of atoms allows the set-up of very specific force models.

The variety of different models which may be calculated with **MODEL1** does not necessarily lead to a complicated mode of operation. Rather, a formalism is found which reduces the required number of input cards as much as possible and, hence, facilitates the use of this program.

The theoretical basis of **MODEL1** is discussed in chapter 2. Here, we only want to give some additional informations which are important for numerical calculations. The entire model is composed on the basis of pair-interactions. Since we deal with central forces, the interactions between two pairs of atoms belonging to the same neighbouring shell are assumed to be identical. This is definitely true if longitudinal and transverse force constants are deduced from a specific interatomic potential. Whenever an interaction is described by atom-specific parameters like a short-range repulsion parameter σ (Born-Mayer potential), a charge Z (Coulomb-potential) or a polarizability α (shell model) the same parameter applies to all atoms of the same type as defined in **GROUP**. The range for the validity of a short-range interaction type is always given in numbers of neighbouring shells since these have already been analyzed by **NN**.

As discussed in sections 2.1 and 2.4 the Dynamical Matrix and the Fourier transformed force constant matrix can be collected from (3×3) submatrices $\mathbf{D}^{(m)}(\kappa\kappa'|\mathbf{q})$ and $\mathbf{F}^{(m)}(\kappa\kappa'|\mathbf{q})$, respectively, which describe the interaction between particles κ and κ' according to the interaction type or model potential m. The shell model, however, requires a hermitian transformation of the full $(3N \times 3N)$ matrices. Here, the Fourier transformed force constant matrices $\mathbf{F}^S$ and $\mathbf{F}^T$, resp. $\mathbf{F}^T$, as defined in section 2.5 must be treated separately and these, in turn, can be collected from small submatrices. Thus, the problem of constructing a Dynamical Matrix is reduced to the calculation of the submatrices $\mathbf{F}(\kappa\kappa'|\mathbf{q})$, $\mathbf{F}^S(\kappa\kappa'|\mathbf{q})$, $\mathbf{F}^T(\kappa\kappa'|\mathbf{q})$ and $\mathbf{C}(\kappa\kappa'|\mathbf{q})$[6]. We can restrict ourselves to those pairs of atoms κ and κ' which correspond to one of the independent interactions determined by program **IND**. Other submatrices are calculated by means of the transformation (2.82) and, since the matrices $\mathbf{F}$ and $\mathbf{F}^S$ are hermitian, $\mathbf{F}(\kappa'\kappa|\mathbf{q})$, $\mathbf{F}^S(\kappa'\kappa|\mathbf{q})$ and $\mathbf{C}(\kappa'\kappa|\mathbf{q})$ are obtained immediately. $\mathbf{F}^T$,

[6] In the present context, $\mathbf{F}$ denotes that part of the Fourier transformed force constant matrix which does not contain polarization effects.

however, may be non-hermitian. Therefore, another independent submatrix, namely $F^T(\kappa'\kappa|q)$ is considered in the program.

Inserting all these small matrices into the full ($3N \times 3N$) matrices and calculating the self terms according to equation (2.6) from the condition of translational invariance, the Fourier transformed force constant matrices are obtained. If the shell model is used, finally the transformation of equation (2.67) is performed and the resultant matrix is combined with **F** and multiplied by the mass tensor to give the complete Dynamical Matrix.

The Coulomb potential is long-ranged and the corresponding part of the Dynamical Matrix is represented by rapidly converging series in direct and reciprocal space according to *EWALD* [5] as discussed in section 2.3. The maximal radius r_{max} for the summation in direct space can be given as input. The Ewald-parameter p corresponding to the width of the Gaussian charge distribution (see equation (2.35)) is calculated from r_{max} by

$$x = r_{max}\sqrt{p} = 4.17 \qquad (4.4)$$

as proposed by *NÜSSLEIN* [9]. This choice is convenient since both damping factors entering in the two series are sufficiently small for this value of x:

$$e^{-x^2} \approx 2.8\ 10^{-8} \quad \text{and} \quad 1 - \mathrm{erf}(x) \approx 3.8\ 10^{-9}.$$

The program checks whether the choice of r_{max} is suitable or not: First, r_{max} should not be too large in order to be able to use the results of program **NN**; *i.e.* r_{max} has to be smaller than the radius of the last neighbouring shell examined in **NN**. Second, if two neighbouring shells are very close to one another, the consideration of only one of these shells may lead to wrong results. In this case, r_{max} will automatically be reduced until a gap of more than 0.5 Å between two shells is reached. If the corresponding radii are d_n and d_{n+1}, r_{max} is calculated as:

$$r_{max} = 0.2\, d_n + 0.8\, d_{n+1}. \qquad (4.5)$$

The actual values used within a calculation can be printed if desired (see control parameters, section 4.4.7).

Note that the phonon wavevector must not be set exactly equal to zero if Coulomb interaction is used (see footnote [2] on page 7 and section 4.1.1)

If the Dynamical Matrix is completed, the symmetry coordinates determined in **GROUP** are used for the block-diagonalization according to equation (2.99). The diagonalization of the individual blocks yields the eigenvalues and eigenvectors. The latter are retransformed to the cartesian coordinate system by multiplication with the symmetry coordinates (equation (2.100)).

4.4.2 The Position of MODEL1 within the Framework of UNISOFT

MODEL1 is the central program of UNISOFT. It uses all the results of programs **GROUP**, **IND** and **NN** which have to be run first. The data are read from the files **COORD** (logical unit 1), **INDDAT** (logical unit 3) and **XNN** (logical unit 4). The calculated Dynamical Matrices, Coulomb coefficients, eigenvectors and eigenvalues may be stored on the disk-dataset **RESULT** (logical unit 2), if desired. Via this dataset the results of the model calculation can be transferred to other programs like **HIST**, **PARDER** or **SF**.

4.4.3 The Structure of MODEL1

A schematic block-diagram of **MODEL1** is given in Figure 4 on page 28.
Obviously, the most specific and complex work is done in the two subroutines GETPAR and DYN2. These routines dealing with the definition of the model and with the set-up of the Dynamical Matrix, respectively, are therefore discussed in separate sections. All the other blocks in Figure 4 represent rather simple activities and need not be described in detail. For the diagonalization of the Dynamical Matrix the standard IMSL routine EIGCH is used which is embedded in subroutine EIGEN. If necessary, it can easily be replaced.

A complete list of all subroutines is given in appendix C.

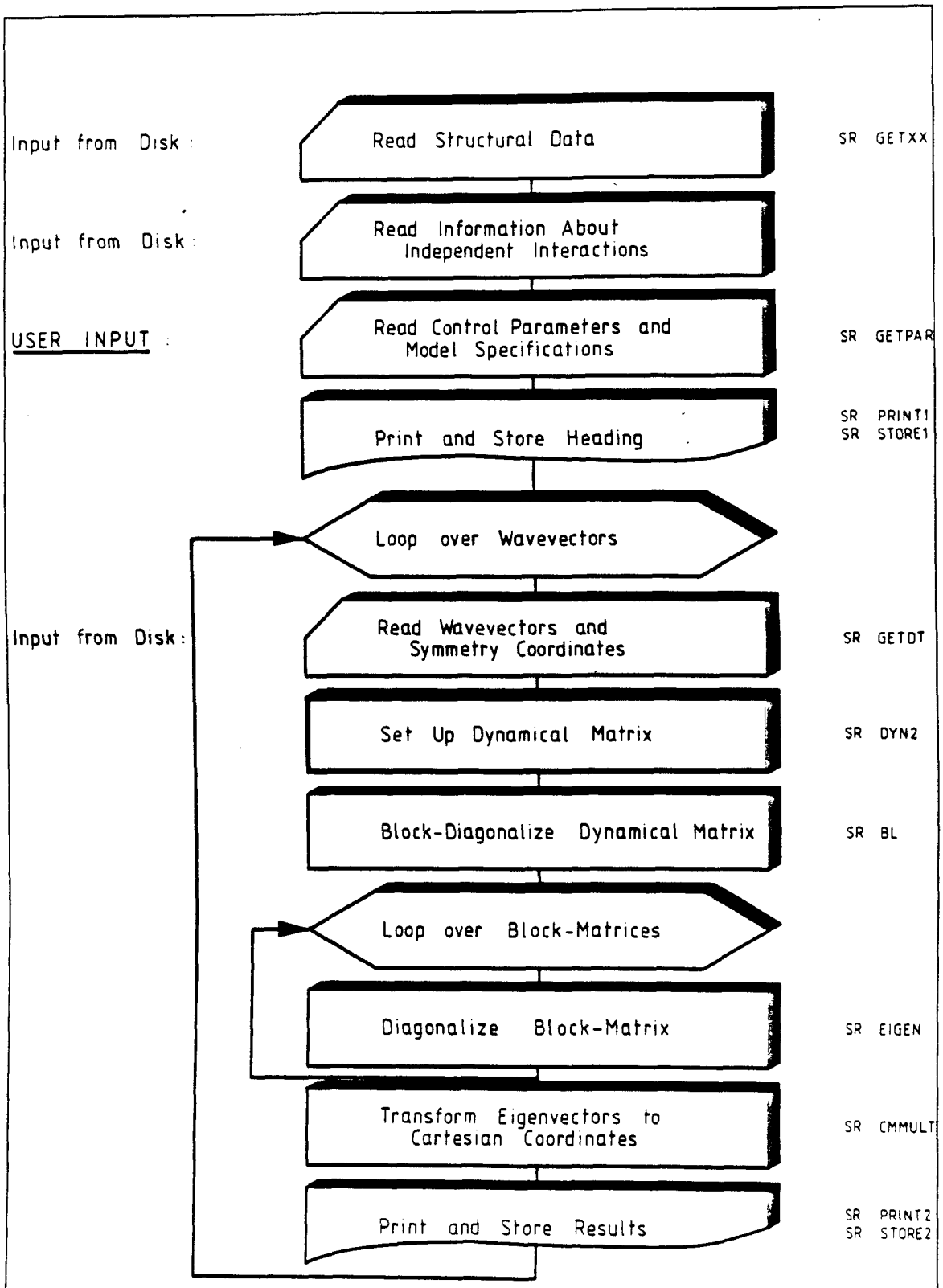

Figure 4. The structure of MODEL1

4.4.4 How to Define a Model Set-Up

In this section the input procedure is described which is governed by subroutine GETPAR. As mentioned earlier, each independent interaction can be modelled by an arbitrary superposition of the different interaction types collected in table 1.

Interaction Type No. Specification	No. of GP's	GP [unit]	No. of ASP's per atom type	ASP [unit]	No. of ISP's per neighb. shell	ISP [unit]
1 Force Constant Model (Born-von Karman)	-		-		2	L [Nm^{-1}] T [Nm^{-1}]
2 Born-Mayer potential	1	V_o [eV]	1	σ [Å]	-	
3 Lennard-Jones potential	1	V_o [eV]	1	σ [Å]	-	
4 van der Waals potential	1	V_o [eV]	1	σ [Å]	-	
5 Coulomb potential	-		1	Z [e]	-	
6 shell model	-		2	Y [e] α [$Å^3$]	6	L^{c-s} [Nm^{-1}] T^{c-s} [Nm^{-1}] L^{s-c} [Nm^{-1}] T^{s-c} [Nm^{-1}] L^{s-s} [Nm^{-1}] T^{s-s} [Nm^{-1}]

V_o	strength of potential
σ	short-range interaction parameter
Z	ionic charge
Y	shell charge
α	free ion polarizability
L	longitudinal force constant
T	transverse force constant

Table 1: Interaction types (model potentials) supported by UNISOFT

Each interaction type is represented by a running number and specified by a certain number of parameters. In order to simplify the input procedure which has to take into account all the different types of interactions, three groups of parameters are introduced:

Atom-Specific Parameters (ASP's)
These parameters depend on the nature of the distinguishable types of atoms only. Examples are the Born-Mayer radius, the ionic charge, the electronic polarizability, etc..

General Parameters (GP's)
These parameters are independent of atomic properties. The prefactors V_o in the Born-Mayer, Lennard-Jones or van der Waals potentials are examples.

Interaction-Specific Parameters (ISP's)

These parameters in general depend on a particular *pair* of atoms and not only on the nature of each individual one. Examples are force constants in the Born-von Karman model or in the shell model. It is assumed that the same ISP's hold for all pairs of atoms κ and κ' which exhibit the same interatomic spacing, *i.e.* for all atoms within the same neighbouring shell.

The corresponding parameters for the individual interaction types supported by UNISOFT are included in table 1 on page 29.

Within the model set-up all the different parameters are labelled by a running integer. Actual values are assigned to the various parameters at the end of the input. Thus different interactions may be described by the same parameters, *e.g.*, and the modification of parameter values is independent of the model set-up.

Example: Suppose you have two pairs of atoms (κ,κ') and (λ,λ') the interaction of which is modelled by longitudinal (L) and transverse (T) springs (Born-von Karman model). These parameters may be labelled by the numbers 1, 2, 3, 4 where the parameters 1 and 2 correspond to L and T for the κ-κ' interaction while the parameters 3 and 4 describe the λ-λ' interaction. After having completed the model set-up for all interactions the actual parameter values are given as a series like:

100. 17. 50. 19. ...

assigning $L(\kappa\kappa') = 100\ Nm^{-1}$, $T(\kappa\kappa') = 17\ Nm^{-1}$, $L(\lambda\lambda') = 50\ Nm^{-1}$ and $T(\lambda\lambda') = 19\ Nm^{-1}$. For the calculation of phonon frequencies for other sets of parameter values only this last line must be modified. If the λ-λ' interaction is to be identical with the κ-κ' interaction (in spite of being symmetrical inequivalent) the same parameter number can be used for both and parameters 3 and 4 are dropped.

The specification of a particular interaction model is achieved in the following manner:

1. **Give the number N of an interaction type.**
2. **Give the numbers for ASP's and GP's for interaction type N, if any.**
3. **Select those pairs of atoms I,J to which the interaction type N is applied and give the number of neighbouring shells NS until which this interaction is extended. (In the case of Coulomb interaction, NS = 5, all atoms in the whole crystal are automatically considered.)**
4. **For each of the NS shells give the numbers for ISP's, if any.**
5. **Repeat steps 3 and 4 until all *independent* pair-interactions are worked through.**
6. **Repeat the whole sequence, 1.-5., for different interaction types until the model set-up is completed.**
7. **Assign values to all the parameters used in the set-up.**

Further examples might illustrate this procedure (the input numbers are printed in bold):

a) Born-von Karman interactions between atoms 1 and 4 up to the second nearest neighbours and between atoms 2 and 5 up to the third nearest neighbours:
Interaction type **1**
No ASP's and GP's
Pair **1 4** considering **2** neighbouring shells
ISP's **1**(L) **2**(T) for the first shell
ISP's **3**(L) **4**(T) for the second shell
Pair **2 5** considering **3** neighbouring shells
ISP's **5**(L) **6**(T) for the first shell
ISP's **7**(L) **8**(T) for the second shell
ISP's **9**(L) **10**(T) for the third shell

If all Born-von Karman interactions are specified a **blank** input card indicates the end of input for interactions of type 1.

b) Born-Mayer potential between atoms 3 and 6 up to the second neighbouring shell and between atoms 4 and 7 for nearest neighbours only. (Suppose you have 4 different types of atoms in the crystal):
Interaction type **2**
Born-Mayer radii σ as ASP's: **11 12 13 14**
Prefactor V_0 as GP: **15**
Applied to pair **3 6** considering **2** shells
No ISP's
Applied to pair **4 7** considering **1** shell
No ISP's

If all Born-Mayer interactions are specified a **blank** input card indicates the end of input for interaction type 2. (The short-range interactions 3 (Lennard-Jones potential) and 4 (van der Waals potential) are treated similarly.)

c) Coulomb potential assuming 4 different atom types:
For the Coulomb potential an extra input card specifying the maximal radius for the summation in direct space has to be given. A proper choice is 5 ... 10 Å.
Interaction type **5**
Maximal radius: **7.5**
Charges as ASP's: **16 16 17 18**
and nothing else, since the Coulomb potential applies to the whole crystal. Note, in this example the same charge, given by parameter 16, is assigned to atoms of type 1 and 2.

d) Shell model:
(If the shell model is required the Coulomb potential has to be specified as well.)
Nearest neighbour atoms 5 and 8 are coupled by the shell model interactions:
Interaction type **6**
ASP's: shell charges **19 19 19 20** and polarizabilities **21 21 21 22**
Pair **5 8** considering **1** shell
ISP's: **23**(L^{c-s}) **24**(T^{c-s}) **23**(L^{s-c}) **24**(T^{s-c}) **25**(L^{s-s}) **26**(T^{s-s})
Again, a **blank** input card indicates the end of input for interaction type 6.
Note, in this example the same charges and polarizabilities are assigned to atoms of type 1, 2 and 3 (given by parameters 19 and 21) and the core-shell and the shell-core coupling between atoms 5 and 8 are identical (given by parameters 23 and 24).

If no other interaction types are needed a further **blank** input card indicates the end of model specification.
Finally, the values for all the parameters (1...26) are given in the corresponding units listed in table 1 on page 29.

It should be noticed again that the specification of a model is to be confined to the independent interactions listed by program **IND**.

The input for program **MODEL1** is completed by a card with output-control parameters and by one or more cards containing the masses of the different types of atoms.

The input is interpreted by the subroutine GETPAR which automatically transfers the specification of a particular interaction to all the symmetrical equivalent ones.

4.4.5 Mode of Parameter-Storage

All parameter numbers used within a particular model set-up are stored one behind the other, just as they are read in, in the integer vector IP. In order to find the correct parameter numbers for one specific interaction during the model calculation there are two pointers to elements of IP:

LOCM(N) points to the location containing the number of the first atom-specific parameter (ASP) of interaction type N.

LOC(I,J,N) points to the location containing the number of neighbouring shells (multiplied by 1000) which are to be considered for the interaction between atom I and J according to interaction type N.

A special subroutine NPM determines the number of ASP's and ISP's for a given interaction type N returning the variables:

NPAR(1,N) = total number of ASP's + total number of GP's
NPAR(2,N) = total number of ISP's per neighbouring shell[7] .

Obviously, the total number of ASP's depends on the number of different atom types determined by program **IND**. The numbers of the NPAR(1,N) atom-specific and general parameters are stored one behind the other on the vector IP starting at location LOCM(N) + 1. Similarly, the numbers of the NPAR(2,N) ISP's for the different neighbouring shells are stored starting at location LOC(I,J,N) + 1.

A schematical representation of the vector IP is given in Figure 5 on page 33.

Note, that the implementation of new interaction types requires the modification of subroutine NPM.

If the interaction between atoms I and J is specified by input and the interaction between IT and JT is symmetrical equivalent it is sufficient to assign

$$LOC(IT,JT,N) = LOC(I,J,N)$$

in order to obtain a proper model set-up. The relation

$$LOC(J,I,N) = LOC(I,J,N) ,$$

however, is not always true: In the shell model the core-shell coupling and the shell-core coupling might be different. In this case, the parameters for the interaction between J and I as deduced from those for the I-J interaction are transferred to an unused location on the vector IP.

The actual value of a parameter entering in the calculation is stored in the real vector P: P(I) is the value of the parameter number I.

The total interaction (as a superposition of different model potentials) between atoms I and J is coded in the array NMOD(I,J) which is defined by

$$NMOD(I,J) = \sum_m w_m 2^{m-1} \qquad (4.6)$$

where the summation runs over all interaction types and w_m = 1 (0) if interaction m is (not) included in the model set-up for the I-J coupling.

4.4.6 Calculation of the Dynamical Matrix

As can be seen from Figure 4 on page 28 the calculation of the Dynamical Matrix is performed in subroutine DYN2. DYN2 itself represents a network of relatively small subroutines each of which dealing with a very specific job. Figure 6 on page 34 displays the overall structure of DYN2.
Within the loop over all pairs of particles I,J the (3 × 3) submatrices corresponding to the I-J interaction are calculated. In a first step, the interaction types are determined in subroutine MODX. The main job is then done by subroutine DIJ which returns the Fourier transformed force constant matrix $\mathbf{F}(IJ|\mathbf{q})$ (= DD)[8], the matrix of Coulomb coefficients multiplied by the charges $\mathbf{F}^C(IJ|\mathbf{q})$ (= CEM) (if the Coulomb potential is invoked) and, in case of the shell model, the matrices $\mathbf{F}^T(IJ|\mathbf{q})$ (= TT), $\mathbf{F}^T(IJ|\mathbf{q})$ (= TT1) and $\mathbf{F}^S(IJ|\mathbf{q})$ (= SS). Furthermore, the corresponding matrices for $\mathbf{q} = 0$ (resp. $\mathbf{q} = \delta\mathbf{q}$ for Coulomb interaction) which enter in the self terms (PP, MST, PTT, PTT1 and PSS) are calculated in DIJ as well. The difference vectors between atoms I and J for the various neighbouring shells are read from the disk-dataset XNN (logical unit 4) and the different interaction types are considered in a do-loop. Decoding the information contained in the vector IP (see section 4.4.5) subroutine GETPM gets the specific parameter values determining the interaction according to one single model potential.

Subroutine MODELX serves as a switch to the different routines performing the calculation for a particular interaction type. Obviously, new model potentials can easily be included just by supplying additional short subroutines at this stage.

---

[7] A value NPAR(2,N) = -1 indicates that there are no ISP's but the particles to which the interaction type N is applied must be specified.

[8] In brackets, the names used in the program listing are given.

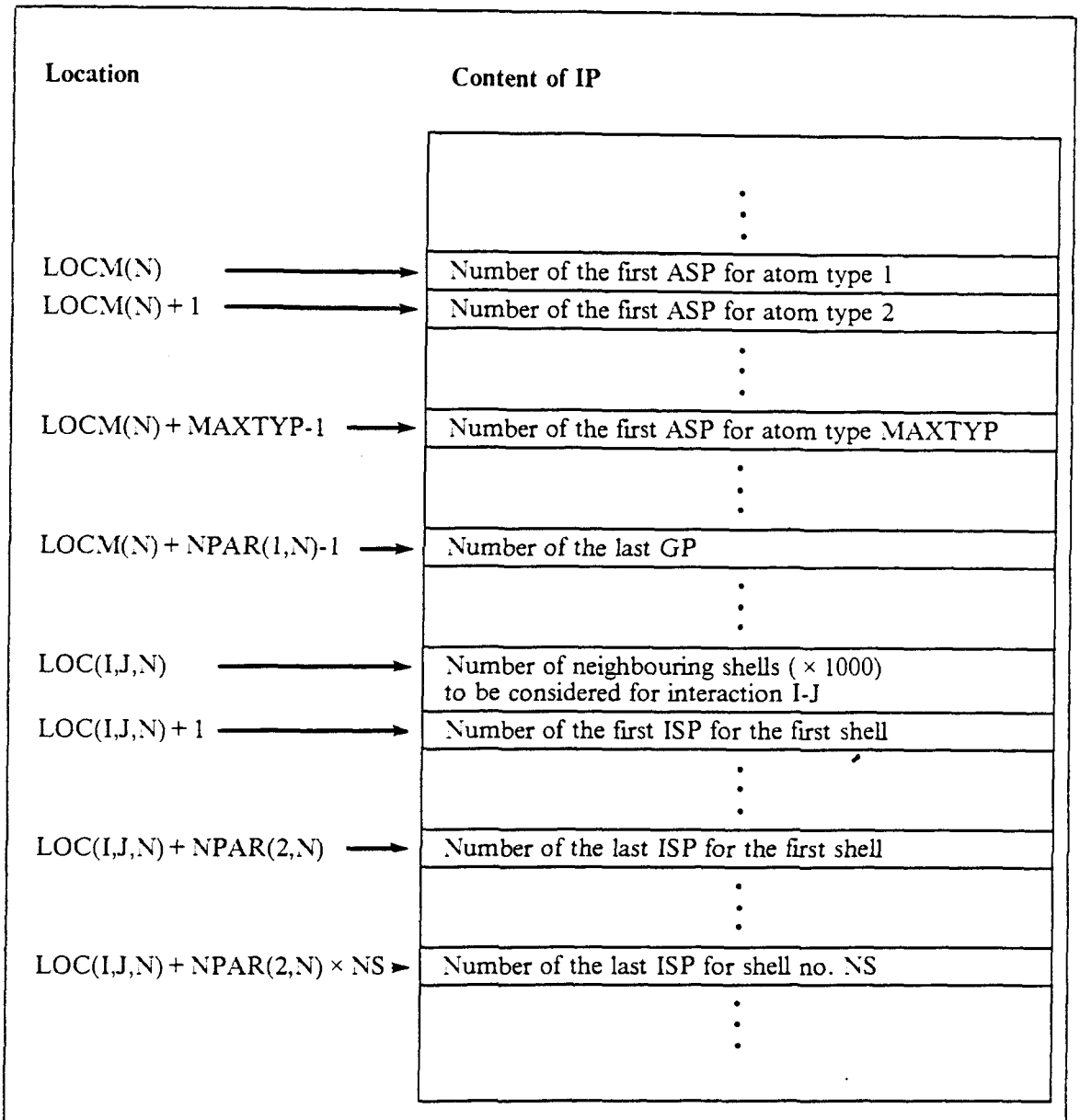

Figure 5. Parameter storage for interaction N within the vector IP

Leaving the subroutine DIJ the matrix elements are rounded; *i.e.* all numbers with moduli smaller than 10^{-20} are set zero. Subroutine CTOD changes the matrices to the D-definition corresponding to equation (2.13) (c.f. footnote [1] on page 4).

The resulting matrices are inserted into the full ($3N \times 3N$) matrices $\mathbf{F}(\mathbf{q})$ (= D), $\mathbf{F}^{C}(\mathbf{q})$ (= C), $\mathbf{F}^{T}(\mathbf{q})$ (= T) and $\mathbf{F}^{S}(\mathbf{q})$ (= S) by subroutine CINS. The same is done for the real $\mathbf{q} = 0$-matrices by subroutine MINS (yielding PH, MC, PT and PS). The symmetrical equivalent interactions are considered in subroutines CTRNSF and MTRNSF according to equation (2.82).

All interactions for which the matrix elements are determined either by direct calculation or by symmetry considerations are labelled by ID(I,J) = 1. Thus, a multiple treatment of the same submatrix is avoided.

For the matrices F (= D) and, if the shell model is used, $\mathbf{F}^{T}$ (= T) and $\mathbf{F}^{S}$ (= S) the self term is calculated from the condition of translational invariance (equation (2.6)) in subroutine SELF. If needed, the polarization part of the Dynamical Matrix, *i.e.* the third term on the right hand side of equation (2.67), is calculated and added to the rest of the Fourier transformed force constant matrix in subroutine SHELL2. Here, for the inversion of the matrix $\mathbf{F}^{SS}$ + YCY the IMSL routine LEQT1C is used which may be replaced if desired.

As the final operation in DYN2, the multiplication with the mass-tensor (in subroutine MDM) yields the complete Dynamical Matrix **D**.

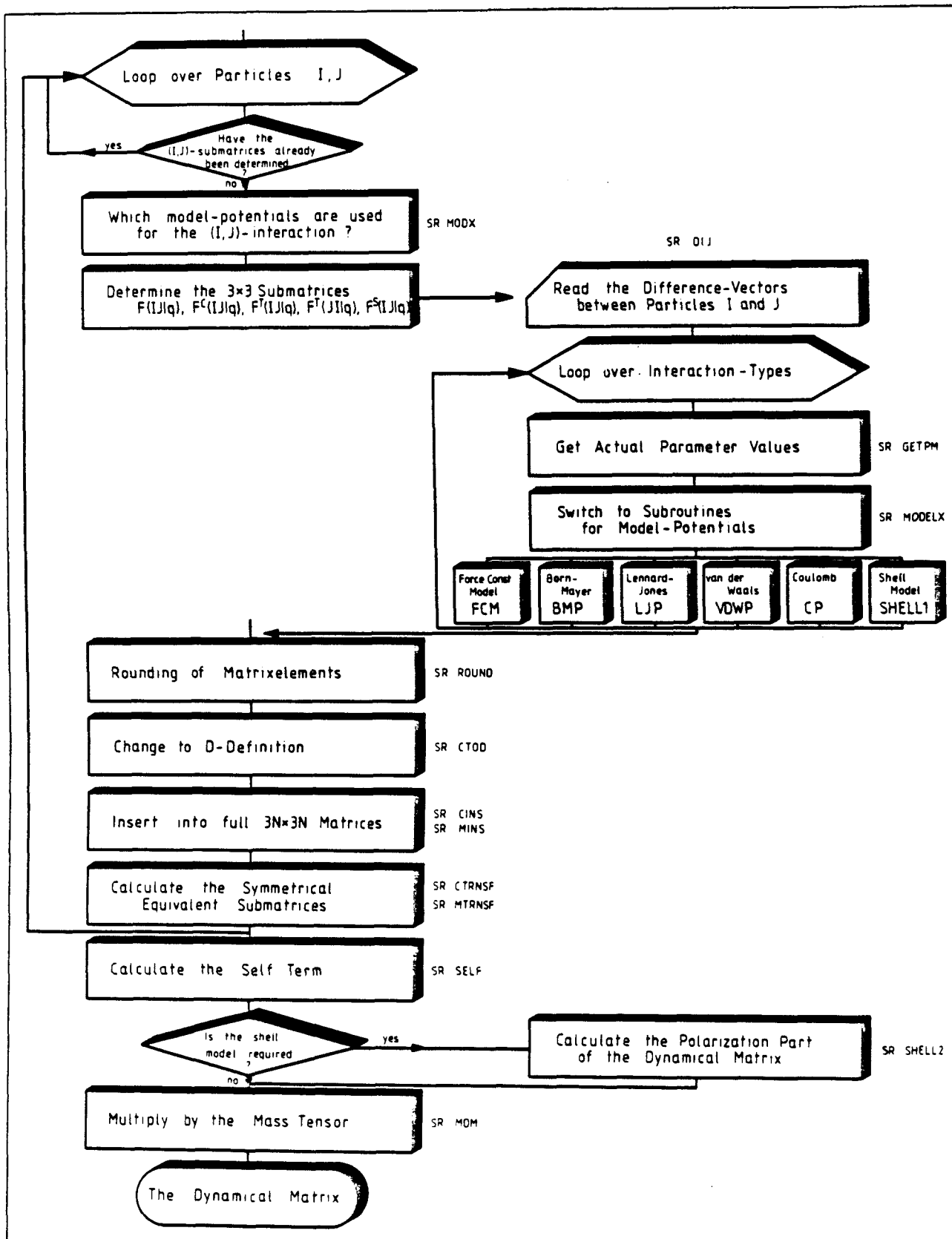

Figure 6. The structure of subroutine DYN2

4.4.7 Input

The idea of the input procedure has already been described in section 4.4.4. Here, we give the specification of the input cards required. A comprehensive list without comment is given in appendix B.3.

Card 1 **(IDIR(I), I = 1,10)** [10I5]

Control parameters:
IDIR(1) = 1(0) (no) printout of symmetry coordinates
IDIR(2) = 1(0) (no) printout of the Dynamical Matrix
IDIR(3) = 1(0) (no) printout the block-diagonalized Dynamical Matrix
IDIR(4) = 1(0) (no) printout the block matrices
IDIR(5) = 1(0) (no) check of diagonalization
IDIR(6) = 1(0) (no) printout of eigenvectors
IDIR(7) = 1(0) (no) printout of parameters for Ewald-summation
IDIR(8) = 1(0) (no) check of translational invariance
IDIR(9) = 1(0) (not) all matrix elements will be calculated independently. Symmetry relations will not be (will be) considered.
IDIR(10) = 1(0) (no) storage of results on disk

Card 2 **(MASS(I), I = 1,MAXTYP)** [8F10.5]

MASS(I) = mass of atom I in atomic mass units
MAXTYP = number of different atom types as determined by program **IND**

Card 3 **N** [I5]

N = Number of interaction type which has to be considered:
N = 1 longitudinal and transverse springs
N = 2 Born-Mayer potential
N = 3 Lennard-Jones potential
N = 4 van der Waals potential
N = 5 Coulomb potential
N = 6 shell model

For Coulomb interaction only:

Card 4 **DMAX** [F10.5]

DMAX = maximal radius in Å for summation in direct space

Only for interaction types containing atom-specific or general parameters (see table 1 on page 29)

Card 5 **((IASP(I,J), J = 1,MAXTYP), I = 1,NASP)**
(IGP(K), K = 1,NGP) [16I5]

MAXTYP = number of different atom types (see program **IND**)
NASP = number of ASP's of interaction N
NGP = number of GP's of interaction N
IASP(I,J) = number of the I-th ASP for atom J
IGP (K) = number of the K-th GP

Not for Coulomb interaction:

Card 6 **I J NS** [3I5]

I, J = number of the atoms between which this interaction N is acting
NS = number of neighbouring shells to be considered

If interaction N contains interaction-specific parameters
(see the table 1) for each of the NS shells a card of the
following type must be given:

Card 7 **(IISP(I), I = 1,NISP)** **[16I5]**
NISP = number of ISP's of interaction N
IISP(I) = number of the I-th ISP of interaction N

Further cards of type 6 and 7
The end of input for the interaction N ($N \neq 5$)
is indicated by a card of type 6 with I = 0

Further interactions may be specified by repeating
the input 3.-7. The end of the model set-up
is indicated by a card of type 3 with N = 0.

Card 8 **(P(I), I = 1,NP)** **[8F10.5]**
NP = largest parameter number used in model set-up (3.-7.)
P(I) = value of parameter number I.

4.4.8 Output

The output is controlled by the vector IDIR (see section 4.4.7). Generally, a list of all interactions within the model set-up is printed by subroutine PRINT1 along with the corresponding parameter numbers and values. By a careful inspection of this list the model can be checked and possible input errors can be detected.

For each value of the wavevector, phonon frequencies $\nu_{qj} = \omega_{qj}/2\pi$ and, if desired, phonon eigenvectors $e(\kappa | qj)$ in cartesian coordinates are listed according to their symmetry (subroutine PRINT2). The wavevectors are printed in cartesian coordinates (in $Å^{-1}$) as well as in units of the reciprocal lattice vectors. An example is given in appendix A.4, page 66.

If needed, the data may be stored on the disk-dataset **RESULT** (logical unit 4) by the subroutines STORE1 and STORE2.

4.5 HIST

4.5.1 General Purpose

The program **HIST** produces a histogram plot of phonon dispersion curves calculated by **MODEL1**. The different branches may be displayed according to their symmetries (irreducible multiplier representations). Obviously, this program can be used in a meaningful way only if the model calculation is performed for a whole sequence of **q**-values. It is, however, not necessary to restrict the wavevectors to a straight line in reciprocal space. Rather, the program recognizes if the sequence corresponds to a zig-zag line. This is especially useful for hexagonal structures, *e.g.*, where normally the phonon dispersion within the hexagonal plane is displayed according to a closed loop of wavevectors: Leaving the Γ-point in direction [100] the zone-boundary is reached at the M-point. On the zone-boundary one can travel from the M- to the K-point from which the Γ-point is approached again in direction [110]. Thus, if the semigraphical representation of phonon frequencies is desired the **q**-values should be carefully selected in program **GROUP**. It should be noticed that the **q**-values need not be of equal distance. The program automatically displays the results according to an absolute scale (except for rounding errors due to the discrete nature of the histogram plot).

There is another criterion for an adequate display of the phonon branches: Suppose, you have more than one irreducible multiplier representation (IMR) of the group of the wavevector for a particular symmetry direction. Then two of them may degenerate at the Γ-point or at the zone-boundary (Z.B.). In this case, it is very illustrative to plot the corresponding branches in an extended zone scheme as may be seen from the following example.

Example In the space group $P6_3$ the main symmetry direction is the hexagonal c-axis. Here, one has six different representations (1 to 6). At the Γ-point IMR 2 is degenerate with IMR 6 and IMR 3 is degenerate with IMR 5, while at the zone-boundary, the A-point, IMR 1 is degenerate with IMR 4, IMR 2 with IMR 3 and IMR 5 with IMR 6. These relations may be checked immediately by inspection of the character tables printed by program **GROUP**. In order to account for the degeneracies it is convenient to plot the dispersion curves according to Figure 7 on page 38.

In fact, the program **HIST** allows to arrange the plot in a very specific way: The sequence of the various irreducible representations can be chosen arbitrarily. The plot direction (Γ → Z.B. or Z.B. → Γ) can be selected by giving the number of the corresponding representation with a positive or a negative sign. In the above example a plot according to Figure 7 on page 38 is obtained by specifying the following sequence of irreducible representations:

```
1   -4   2   -3   5   -6
```

If this sequence starts with 0, all phonon branches are plotted in one picture and different symbols are used to distinguish between the irreducible multiplier representations.

The program **HIST** needs the output results of **GROUP**, **IND** and **MODEL1** which are read from the disk-datasets **COORD** (logical unit 1), **INDDAT** (logical unit 3) and **RESULT** (logical unit 2), respectively.

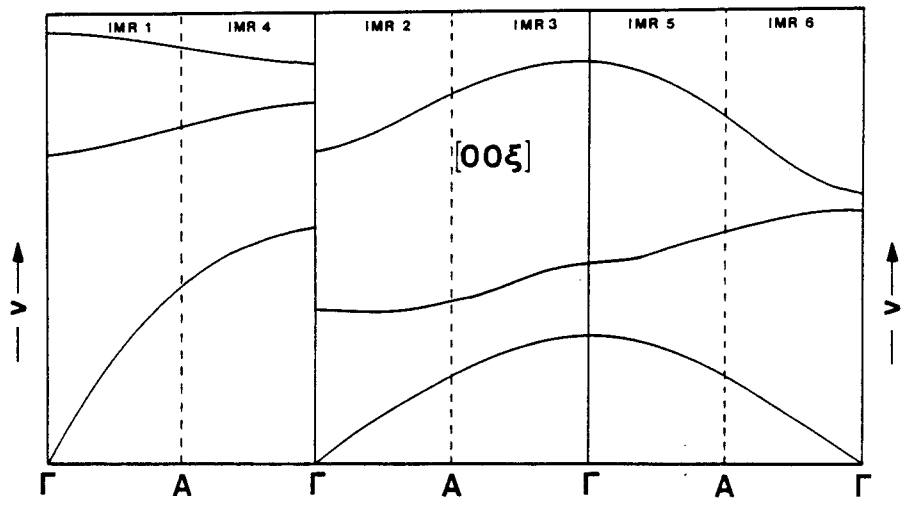

Figure 7. **Schematical illustration of a phonon dispersion:** For the hexagonal direction of the cyclic space group $P6_3$ the dispersion is displayed conveniently according to the different symmetries taking into account the degeneracies at special points within the Brillouin zone.

4.5.2 Input

Card 1 **NYMAX** [F10.6]
NYMAX = maximum frequency in THz

Card 2 **(IDIR(I), I = 1,20)** [16I5]
This is a double card !

IDIR(1),IDIR(2)... is the sequence of irreducible representations to be displayed
If IDIR(I) > 0 the corresponding dispersion curves are plotted from Γ-point towards the zone boundary.
If IDIR(I) < 0 the corresponding dispersion curves are plotted from the zone boundary towards Γ-point.
If IDIR(1) = 0 plot without consideration of symmetry

Card 3 **NMARK** [I5]
selects the symbol used for phonons
NMARK = 1 : *
2 : +
3 : 0
4 : #
5 : @
6 : .
7 : &
8 : $
9 :
10 : X

4.5.3 Output

An example for an output is given in appendix A.5, page 77. It should be noticed again that the quality of the plot obtained by **HIST** depends on a proper choice of the q-values and of the sequence of representations. The display according to the different symmetries has the advantage that the calculated points can immediately be joined by lines corresponding to the different phonon branches since there is no intersection of branches (except at points of higher symmetry).

4.6 SF

4.6.1 General Purpose

The experimental determination of phonon dispersion curves by neutron scattering can effectively be supported by model calculations. The phonon intensities are given by the dynamical structure factor as discussed in section 2.8. Model calculations do not only yield the eigenfrequencies but also the eigenvectors of lattice vibrations and, hence, the intensity for any particular phonon can be predicted.

The program **SF** calculates the dynamical structure factors on the basis of the lattice-dynamical model considered in program **MODEL1**. According to equation (2.95) the expression

$$F\left|\sum_{\kappa}\frac{b_\kappa}{\sqrt{m_\kappa}}e^{-W_\kappa}(g+q)e(\kappa|qj)\right|^2 \tag{4.7}$$

is listed for any phonon mode j and for a specified range of Brillouin zones g. F is a normalizing factor which can be chosen arbitrarily in order to get reliable numbers on output. If desired, the $1/\omega_{qj}$-factor or the Bose-occupation factor n_{qj} are included. The Debye-Waller factor e^{-W_κ} is calculated as:

$$e^{-W_\kappa} = e^{-\frac{1}{2}(g+q)B_\kappa(g+q)}, \tag{4.8}$$

where $\mathbf{B}_\kappa$ is the symmetrical matrix of anisotropic temperature factors:

$$\mathbf{B}_\kappa = \begin{pmatrix} TF_\kappa(1) & TF_\kappa(2) & TF_\kappa(3) \\ TF_\kappa(2) & TF_\kappa(4) & TF_\kappa(5) \\ TF_\kappa(3) & TF_\kappa(5) & TF_\kappa(6) \end{pmatrix}. \tag{4.9}$$

This matrix has to be given as input as well as the coherent scattering lengths b_κ. It is, however, sufficient to specify $\mathbf{B}_\kappa$ and b_κ for only one atom of each type. The temperature factors of all other atoms of the same type are obtained by a simple matrix transformation.

The output list can be arranged according to irreducible multiplier representations or according to increasing frequencies. The most convenient choice depends on the specific crystal system under consideration.

The results obtained by programs **GROUP**, **IND** and **MODEL1** are used via the disk-datasets **COORD** (logical unit 1), **INDDAT** (logical unit 3) and **RESULT** (logical unit 2), respectively.

4.6.2 Input

The range of Brillouin zones for which the dynamical structure factors are calculated is determined by the lower and upper limits for the Miller indices (HMIN, HMAX, KMIN, KMAX, LMIN, LMAX) as well as by a limiting radius QMAX which is to be given in $Å^{-1}$. In particular, the following cards are required for the program **SF**:

Card 1 **HMIN, HMAX, KMIN, KMAX, LMIN, LMAX** [6I5]
define the range of Brillouin-zones for which phonon intensities are calculated:
HMIN ≤ h ≤ HMAX
KMIN ≤ k ≤ KMAX
LMIN ≤ l ≤ LMAX

Card 2 **QMAX** [F10.6]
QMAX = maximum value for **q** in $Å^{-1}$ limiting the range of Brillouin zones

Card 3 **(B(I), I = 1,MAXTYP)** [8F10.6]
B(I) = coherent scattering length in 10^{-14} m for atoms of type I
MAXTYP = number of different particle types as determined by program **IND**

For each of the MAXTYP types of particles a card of the following type must be given:

Card 4 **I, (TF(K), K = 1,6)** [I5,6F10.6]
I = number of atom (representing the class of corresponding type)
TF(K) = components of the tensor B of anisotropic temperature factors in $Å^{-2}$ (see equation (4.9))

Card 5 **T** [F10.6]
T = temperature in K

Card 6 **FNORM** [F10.6]
FNORM = normalizing factor.

Card 7 **(IDIR(I), I = 1,10)** [10I5]
Control parameters:
IDIR(1) = 1 : output arranged according to irreducible representations
IDIR(1) = 2 : output arranged according to frequency scale
IDIR(4) = 1(0) : calculations (do not) take into account 1/v-factor
IDIR(5) = 1(0) : calculations (do not) take into account Bose-factor

4.6.3 Output

An output example is given in appendix A.6, page 79. The list may serve as a guide for neutron scattering experiments: For a particular phonon, a Brillouin zone is picked out where its intensity is large and, simultaneously, the intensities of neighbouring phonons (on the frequency scale) are sufficiently small. If the lattice-dynamical model is adequate the phonon under consideration should be very well detected in this particular Brillouin zone.

4.7 PARDER

4.7.1 General Purpose

The program **PARDER** calculates the partial derivatives of phonon frequencies with respect to each of the model parameters. It can thus be used for the optimization of a particular lattice-dynamical model.

If **p** denotes the parameter vector determining the Dynamical Matrix the squares of phonon frequencies are represented by:

$$\begin{pmatrix} \omega_1^2 & & \\ & \ddots & \\ & & \omega_{3N}^2 \end{pmatrix} = \mathbf{E}^{+}\mathbf{D}(\mathbf{p})\mathbf{E}\,, \tag{4.10}$$

where **E** is the matrix of the eigenvectors. All matrices appearing in equation (4.10) are determined by program **MODEL1**. If the parameter vector is altered by $\Delta\mathbf{p}$ a new Dynamical Matrix $\mathbf{D}(\mathbf{p} + \Delta\mathbf{p})$ is obtained and, to first approximation, the new phonon frequencies are given by:

$$\begin{pmatrix} \bar{\omega}_1^2 & & \\ & \ddots & \\ & & \bar{\omega}_{3N}^2 \end{pmatrix} = \mathbf{E}^{+}\mathbf{D}(\mathbf{p} + \Delta\mathbf{p})\mathbf{E}\,. \tag{4.11}$$

The variations in ω^2 are:

$$\begin{pmatrix} \Delta\omega_1^2 & & \\ & \ddots & \\ & & \Delta\omega_{3N}^2 \end{pmatrix} = \mathbf{E}^{+}[\mathbf{D}(\mathbf{p} + \Delta\mathbf{p}) - \mathbf{D}(\mathbf{p})]\,\mathbf{E}\,. \tag{4.12}$$

The corresponding shifts of the frequencies ω_i are calculated as:

$$\Delta\omega_i = \frac{\Delta\omega_i^2}{2\omega_i} \qquad \text{if } \omega_i > 0 \tag{4.13}$$

and

$$\Delta\omega_i = \sqrt{\Delta\omega_i^2} \qquad \text{if } \omega_i = 0\,. \tag{4.14}$$

The values $\Delta\nu_i = \Delta\omega_i/2\pi$ are listed for all phonons calculated by **MODEL1** and for variations of all model parameters. Note, that a negative squared frequency ω_i^2 or ν_i^2 obtained by program **MODEL1** is treated as being zero. If, however, the frequency is less or equal zero and, simultaneously, the shift of its square, $\Delta\nu^2$, is calculated to be negative, $\Delta\nu$ cannot be obtained. In this case, $\Delta\nu^2$ itself is listed and a corresponding message is printed.

The individual variations of the different model parameters for which the frequency shifts are calculated are given as input.

As can be seen from equation (4.12) the main task within **PARDER** is to compute a new Dynamical Matrix with slightly modified parameter values. Remembering the modular set-up of the program **MODEL1**, it is obvious that the subroutine DYN2 can be used within **PARDER** as well. Therefore, **PARDER** itself turns out to be a rather simple program constructed around the general subroutine DYN2.

The output list illustrates the effect of each of the model parameters on each phonon frequency. It may serve as a guide if the model has to be modified in order to reproduce the experimental results.

The results of the programs **GROUP**, **IND**, **NN** and **MODEL1** are used via the disk-datasets **COORD** (logical unit 1), **INDDAT** (logical unit 3), **XNN** (logical unit 4) and **RESULT** (logical unit 2), respectively.

4.7.2 Input

In analogy with program **MODEL1** a control card is used to select the mode of computing the Dynamical Matrix:

Card 1 **(IDIR(I), I = 1,10)** **[10I5]**

IDIR(7) = 1(0) : (no) printout of parameters for Ewald-summation

IDIR(9) = 1(0) : (not) all of the matrix elements of **D** will be calculated independently. Symmetry relations will not be (will be) considered.

Card 2 **(DP(I), I = 1,NP)** **[8F10.6]**

Variation of parameter values for which the frequency shifts are calculated NP is the total number of parameters for the model specified in program **MODEL1**.

4.7.3 Output

An example for an output list is given in appendix A.7, page 81. Note that all frequencies calculated in **MODEL1** as being imaginary ($\nu^2 < 0$) are denoted by $\nu = 0.0$ THz. If the frequency is imaginary or zero and the shift of ν^2 is negative, $\Delta\nu^2$ is listed instead of $\Delta\nu$. A corresponding message is printed on the previous output page.

4.8 ROTINV

4.8.1 General Purpose

The program **ROTINV** provides a test of the rotational invariance condition as discussed in section 2.6.2. For a particular lattice-dynamical model the net forces are calculated which act upon the different atoms if the crystal as a whole is rotated around the x-, y- or z-axis. These forces should be zero for a proper model set-up. They can be calculated from the Dynamical Matrix taken at wavevectors δq along different directions near the Γ-point as expressed by equations (2.76)-(2.78). For numerical calculations the modulus δq of the wavevectors has to be chosen carefully: If it is too large the approximation of equation (2.72) may become invalid and, consequently, the results are incorrect. If, on the other hand, δq is too small rounding errors may come into play. The following two conditions can be used as criteria for a proper choice of δq:

1. The component of the force along the direction of rotation $f_\alpha^\alpha(\kappa)$ vanishes for every atom κ in the case of central forces. Thus, the calculated numerical values for f_α^α can be regarded as a monitor of rounding errors.

2. The two components f_α^β and $-f_\beta^\alpha$ of the force tensor have to be identical, irrespective of the special model. The force tensor is antisymmetrical. Again, numerical differences show the influence of rounding errors.

The model to be tested by **ROTINV** is defined in just the same manner as in program **MODEL1**. Thus, the same subroutines are used for the interpretation of input (GETPAR) as well as for the calculation of the Dynamical Matrix (DYN2) (*cf.* section 4.4). Having these routines available, **ROTINV** is a rather simple and straightforward program.

Obviously, **ROTINV** uses all results of the programs **GROUP**, **IND** and **NN** just as **MODEL1** does.

Within one run of **ROTINV**, a particular model set-up can be analyzed for different sets of parameter values. Thus, it can be used to select a proper parameter set (leading to a rotational invariant model) prior to the actual model calculation.

4.8.2 Input

The following input card are required:

Card 1 **QL** **[F10.6]**

QL = modulus of the wavevector δq used for the calculation.
It should be small enough to be sure that the approximation (2.72) is valid.
On the other hand, QL should not be too small because of rounding errors.

Card 2-9 are the same as *Cards 1-8* for program **MODEL1**
The control variable IDIR(1), however, has a different meaning:
IDIR(1) = 1(0) : (no) printout of model specifications

Other parameter sets may be considered by supplying additional cards of type 9 (i.e. type 8 of **MODEL1**).

4.8.3 Output

An example for the output of program **ROTINV** is given in appendix A.8, page 83. The net forces are given in units of 10^{-10} N. A particular model can be regarded as being nearly rotational invariant if the moduli of all force components are smaller than 0.01 10^{-10} N . Rounding errors may be detected by checking the conditions $f_{\alpha}^{\alpha} = 0$ and $f_{\alpha}^{\beta} = -f_{\beta}^{\alpha}$.

4.9 EFG

4.9.1 General Purpose

The program **EFG** calculates local static electrical fields and field gradients for a given structure according to equations (2.103) and (2.104), section 2.10. The lattice sum is evaluated by Ewald's method in just the same way as for the dynamical model calculations. In fact, the electrical field gradients are proportional to a sum over Coulomb coefficients which are calculated by subroutine CP dealing with the Coulomb potential (see Figure 6 on page 34). The same subroutine is therefore used in **EFG** as well. Note, however, that the self-potential has to be excluded. Obviously, the calculations have to be performed for zero wavevector since we are dealing with static properties. In practice, however, **q** is a small but non zero vector in order to overcome the difficulties in numerical calculations mentioned earlier (see footnote [2] on page 7).

Concerning the components of the electrical field, equation (2.104), the method of summation is the same as for the determination of the Coulomb coefficients, except the $\mathbf{g} = 0$ term is excluded. This term comes into play for dynamical calculations only, since lattice vibrations carry a macroscopic electrical field if they are polarized in longitudinal direction.

If desired, the contributions of the different sublattices (containing all atoms of the same type) to the Coulomb force acting upon any particular ion can be listed individually. Thus, partial Madelung constants are obtained if unit charges are considered.

The structural parameters used for the calculations in **EFG** are read from the disk-datasets **COORD** (logical unit 1), **INDDAT** (logical unit 3) and **XNN** (logical unit 4). Thus the programs **GROUP**, **IND** and **NN** have to be run first. As in program **MODEL1** the ordered arrangements of atoms in neighbouring shells provided by program **NN** are used to simplify the summation in direct space. The maximal radius is given as input and is automatically modified by the program, if necessary (*cf.* section 4.4.1). The final parameters for the Ewald-summation may be printed.

4.9.2 Input

The following input cards are required for program **EFG**:

Card 1 **(IDIR(I), I = 1,10)** **[10I5]**
Control parameters:
IDIR(1) = 1(0) : (no) printout of the contributions of the different sublattices to the total Coulomb force
IDIR(7) = 1(0) : (no) printout of parameters for Ewald summation

Card 2 **(Z(I), I = 1,MAXTYP)** **[8F10.6]**
Z(I) = charge of ions of type I in units of the elementary charge
MAXTYP = number of different atom types as determined by program **IND**

Card 3 **DMAX** **[F10.6]**
DMAX = maximal distance for summation in direct space in Å

4.9.3 Output

An example for the output of the program **EFG** is given in appendix A.9, page 85. The components of the local electrical field are given in units of $VÅ^{-1}$, those of the field gradient tensor are given in units of $VÅ^{-2}$.

5.0 Computer Requirements

UNISOFT is written in the FORTRAN IV programming language supported by the most computers. Special features which might be specific to a particular computer system are avoided. Three subroutines are used from the IMSL-library:

1. the random number generator GGUBS used within **GROUP**
2. the diagonalization routine EIGCH for a complex hermitian matrix called by subroutine EIGEN within **MODEL1**
3. the routine LEQT1C for the inversion of a hermitian matrix called by subroutine SHELL2 within **MODEL1**, **ROTINV** and **PARDER**.

If UNISOFT is to be installed at a computer which does not support the IMSL-routines, these subroutines have to be replaced.

The data transfer between the different programs is achieved via the four disk-datasets **COORD**, **INDDAT**, **XNN** and **RESULT** by formatted sequential input and output. Before UNISOFT can be used, these files must be installed. The required sizes of the datasets depend on the crystal structure to be considered. It can be estimated as follows: Suppose, you have a crystal structure with N particles per primitive cell and the calculations are to be performed for M values of the phonon wavevector. Then, the following storage capacities are needed:

COORD	$145 + N + M(9 + 2.25N^2)$ records
INDDAT	28 records
XNN	$60(N^2 + N)$ records
RESULT	$484 + M(4 + 0.6N + 13.5N^2) \approx 500 + 14MN^2$ records.

([X] denotes the smallest integer larger than X.) The logical record length is 80 bytes.

It should be mentioned that UNISOFT is not optimized with respect to storage capacity or with respect to computing time. The main attention has been paid to an easy mode of operation.

6.0 Possible Extensions of UNISOFT

Discussing possible extensions of UNISOFT, one has to distinguish between extensions concerning the lattice-dynamical model on the one hand, and extensions concerning other physical implications of a given model on the other hand.

As already mentioned in section 4, it is rather simple to implement new types of pair interactions. In principle, also tensor forces should be feasible.

The consideration of anharmonic effects obviously requires a more complex treatment. On the basis of the perturbation theory it should, however, be possible to calculate frequency shifts and phonon line widths. In general, this procedure leads to a summation over a large number of phonon states within the whole Brillouin zone. Thus, the computing time for those calculations will become large, especially if the crystal structure under consideration is not a simple one.

The introduction of the concept of molecular groups can also provide a useful extension of the present system: In many crystalline solids there are molecular groups which, from the lattice-dynamical point of view, can be considered as nearly rigid bodies. Thus, not all atoms have to be treated individually. Rather, the dynamics of an entire molecular group, such as SO_4, CH_4, NH_4 etc. can be described by three translational and three rotational degrees of freedom. This approach is justified, if the frequencies of the internal vibrations of a molecular group are much larger than the frequencies of the lattice modes. By the introduction of this concept of molecular crystals obviously the dimension of the Dynamical Matrix and, hence, the computing time can be reduced.

On the basis of a given lattice-dynamical model other physical properties of a crystal may be calculated by adding new programs: Phonon densities of state, *e.g.*, can be calculated if the phonon frequencies have been determined by **MODEL1** for a large number of **q**-values distributed all over the Brillouin zone. In a next step, the contribution of lattice vibrations to the specific heat can be deduced from the phonon density of states. Lattice energies can be calculated. And there are certainly more possible extensions of UNISOFT.

In principle, it is also possible to use **MODEL1** within a least-squares fit program which adjusts the calculated phonon frequencies to measured ones. Often, however, the experimental assignment of phonon peaks to phonon branches is rather difficult. A wrong labelling of a phonon might have fatal consequences: The fitting procedure can lead to definitely wrong results, especially if more complicated crystal structures are considered.

7.0 References

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Appendix A. Example for the Application of UNISOFT

As an example all programs of UNISOFT are applied to the room temperature phase of $KLiSO_4$ which belongs to the space group $P6_3$. In fact, the crystal structure is disordered which can, however, be neglected for lattice-dynamical considerations.

The input data are given along with an excerpt of the resulting output list for each of the individual programs. The complete listings are too voluminous in order to be presented here.

A.1 GROUP

INPUT

```
 GROUP THEORETICAL ANALYSIS OF THE K LI SO4-STRUCTURE
   14    1    0    3    0
K1  K2  LI1 LI2 S1  S2  01  05  02  06  03  07  04  08
 UNIT 1 = K1;       UNIT 2 = K2 ;       UNIT 3 = LI1 ;      UNIT 4 = LI2;
 UNIT 5 = S1;       UNIT 6 = S2 ;
 UNIT 7 = O1;       UNIT 8 = O5;        UNIT 9 = O2;        UNIT 10 = O6;
 UNIT 11 = O3;      UNIT 12 = O7;
 UNIT 13 = O4;      UNIT 14 = O8;

5.142    .000   0.000   -2.571  4.453   0.000   0.000   0.000   8.624
    1  0.         0.        0.        000
    1  0.         0.        4.312     000
    2  0.         2.96874   5.882     000
    2  2.571      1.48437   1.570     000
    3  0.         2.96874   2.535     000
    3  2.571      1.48437   6.847     000
    4 0.          2.9687    3.9670      0
    4 2.5710      1.4844    8.2790      0
    5 1.3909      2.9257    2.0611      0
    5 1.1801      1.5274    6.3731      0
    5 4.4838      4.1948    2.0611      0
    5 3.2292      0.2583    6.3731      0
    5 4.4093      1.7857    2.0611      0
    5 3.3037      2.6674    6.3731      0
.7055     .7055     .7055
   1    0
 GAMMA-POINT
 .000     0.00000      0.00010
   1    1
 0 0 1 -DIRECTION
 .000     0.00000   0.20000
   1    2
 0 0 1 -DIRECTION
 .0000    0.000000  0.400
   0    0
```

OUTPUT

```
GROUP THEORETICAL ANALYSIS OF THE K LI SO4-STRUCTURE
UNIT 1 = K1;        UNIT 2 = K2 ;       UNIT 3 = LI1 ;      UNIT 4 = LI2; NIT 5 = S1;       UNIT 6 = S2 ;
UNIT 7 = O1;        UNIT 8 = O5;        UNIT 9 = O2;        UNIT 10 = O6;NIT 11 = O3;       UNIT 12 = O7;
UNIT 13 = O4;       UNIT 14 = O8;

                RECIPROCAL SPACE LATTICE VECTORS                    POSITION VECTOR SPACE LATTICE VECTORS
                    A1(I)*A(J)=DELTA(I,J)                                A1              A2              A3
          A11= (  0.19448,  0.11228,  0.0     )              (   5.14200 ) ( -2.57100 ) (  0.0     )
          A12= (  0.0     ,  0.22457,  0.0     )              (   0.0     ) (  4.45300 ) (  0.0     )
          A13= (  0.0     ,  0.0     ,  0.11596)              (   0.0     ) (  0.0     ) (  8.62400 )


THE CRYSTAL SYSTEM IS HEXAGONAL    WITH OPERATIONS:  1  2  3  4  5  6

THE SPACE GROUP IS NON-SYMMORPHIC OR ELSE A NON STANDARD ORIGIN OF COORDINATES WAS USED.

                                                                ATOM TRANSFORMATION TABLE
                                                    OPERATION NUMBER    1  2  3  4  5  6
MOVES ATOM  1 TYPE  1 AT ( 0.0    , 0.0    , 0.0    ) TO ATOM    1  2  1  2  1  2
MOVES ATOM  2 TYPE  1 AT ( 0.0    , 0.0    , 4.3120) TO ATOM    2  1  2  1  2  1
MOVES ATOM  3 TYPE  2 AT ( 0.0    , 2.9687, 5.8820) TO ATOM    3  4  3  4  3  4
MOVES ATOM  4 TYPE  2 AT ( 2.5710, 1.4844, 1.5700) TO ATOM    4  3  4  3  4  3
MOVES ATOM  5 TYPE  3 AT ( 0.0    , 2.9687, 2.5350) TO ATOM    5  6  5  6  5  6
MOVES ATOM  6 TYPE  3 AT ( 2.5710, 1.4844, 6.8470) TO ATOM    6  5  6  5  6  5
MOVES ATOM  7 TYPE  4 AT ( 0.0    , 2.9687, 3.9670) TO ATOM    7  8  7  8  7  8
MOVES ATOM  8 TYPE  4 AT ( 2.5710, 1.4844, 8.2790) TO ATOM    8  7  8  7  8  7
MOVES ATOM  9 TYPE  5 AT ( 1.3909, 2.9257, 2.0611) TO ATOM    9 14 11 10 13 12
MOVES ATOM 10 TYPE  5 AT ( 1.1801, 1.5274, 6.3731) TO ATOM   10 13 12  9 14 11
MOVES ATOM 11 TYPE  5 AT ( 4.4838, 4.1948, 2.0611) TO ATOM   11 10 13 12  9 14
MOVES ATOM 12 TYPE  5 AT ( 3.2292, 0.2583, 6.3731) TO ATOM   12  9 14 11 10 13
MOVES ATOM 13 TYPE  5 AT ( 4.4093, 1.7857, 2.0611) TO ATOM   13 12  9 14 11 10
MOVES ATOM 14 TYPE  5 AT ( 3.3037, 2.6674, 6.3731) TO ATOM   14 11 10 13 12  9
                                                    MULTIPLICATION TABLE,30X,23HFRACTIONAL TRANSLATIONS
      1  2  3  4  5  6
   1  1  2  3  4  5  6
   2  2  3  4  5  6  1
   3  3  4  5  6  1  2
   4  4  5  6  1  2  3
   5  5  6  1  2  3  4
   6  6  1  2  3  4  5
THE CARTESIAN AXES INTERSECT THE BRILLOUIN ZONE BOUNDARIES AT ( 0.81463, 0.70550, 0.36428)
THE INPUT WAVE VECTORS WILL BE SCALED BY                      ( 0.70550, 0.70550, 0.36428)
**********************************************************************************************************************

GROUP THEORETICAL ANALYSIS OF THE K LI SO4-STRUCTURE
GAMMA-POINT
**********************************************************************************************************************

K IS ONE HALF OF A WAVE VECTOR SPACE LATTICE VECTOR, THEREFORE THE DYNAMICAL MATRIX MUST BE REAL.
----------------------------------------------------------------------------------------------------------------------
                                                    CHARACTER TABLE

OP     IR( 1)     IR( 2)     IR( 3)     IR( 4)     IR( 5)     IR( 6)
 1    1.0 -0.0  1.0 -0.0  1.0 -0.0  1.0 -0.0  1.0 -0.0  1.0 -0.0
 2    1.0 -0.0  0.5 -0.9 -0.5 -0.9 -1.0  0.0 -0.5  0.9  0.5  0.9
 3    1.0 -0.0 -0.5 -0.9 -0.5  0.9  1.0 -0.0 -0.5 -0.9 -0.5  0.9
 4    1.0 -0.0 -1.0  0.0  1.0 -0.0 -1.0  0.0  1.0 -0.0 -1.0  0.0
 5    1.0 -0.0 -0.5  0.9 -0.5 -0.9  1.0 -0.0 -0.5  0.9 -0.5 -0.9
 6    1.0 -0.0  0.5  0.9 -0.5  0.9 -1.0  0.0 -0.5 -0.9  0.5 -0.9
IMR NUMBER  6 IS TIME REVERSAL DEGENERATE WITH IMRNUMBER  2.  IN THE DECOMPOSITION IMR  6 WILL BE DROPPED
AND IMR  2 WILL HAVE TWICE THE DIMENSION IT HAD.
IMR NUMBER  5 IS TIME REVERSAL DEGENERATE WITH IMRNUMBER  3.  IN THE DECOMPOSITION IMR  5 WILL BE DROPPED
AND IMR  3 WILL HAVE TWICE THE DIMENSION IT HAD.
----------------------------------------------------------------------------------------------------------------------
   THE DECOMPOSITION IS  7 IR( 1) +  7 IR( 2) +  7 IR( 3) +  7 IR( 4)
----------------------------------------------------------------------------------------------------------------------
```

SYMMETRY REDUCED DYNAMICAL MATRIX.

THE NUMBER OF INDEPENDENT ELEMENTS IS LARGER THAN EXPECTED FROM THE DECOMPOSITION FORMULA, I.E., 334 .GT. 112.

AMPLITUDES

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	AA	..	..	AB	..	..	AC	AD	..	AE	AF	..	AG	AH	..	AI	AJ	..	AK	AL	..	AM	AN	..	AO	AP	AQ	AR	AS	AT
2	..	AA	..	..	AB	..	AD	AC	..	AF	AE	..	AH	AG	..	AJ	AI	..	AL	AK	..	AN	AM	..	BG	BH	BI	BJ	BK	BL
3	..	..	BY	..	..	BZ	..	..	CA	..	..	CB	..	..	CC	..	..	CD	..	..	CE	..	..	CF	CG	CH	CI	CJ	CK	CL
4	AB	..	..	AA	..	..	AE	AF	..	AC	AD	..	AI	AJ	..	AG	AH	..	AM	AN	..	AK	AL	..	AR	AS	AT	AO	AP	AQ
5	..	AB	..	..	AA	..	AF	AE	..	AD	AC	..	AJ	AI	..	AH	AG	..	AN	AM	..	AL	AK	..	BJ	BK	BL	BG	BH	BI
6	..	..	BZ	..	..	BY	..	..	CB	..	..	CA	..	..	CD	..	..	CC	..	..	CF	..	..	CE	CJ	CK	CL	CG	CH	CI
7	AC	AD	..	AE	AF	..	CU	..	..	CV	..	..	CW	CX	..	CY	CZ	..	DA	DB	..	DC	DD	..	DE	DF	DG	DH	DI	DJ
8	AD	AC	..	AF	AE	..	..	CU	..	..	CV	..	CX	CW	..	CZ	CY	..	DB	DA	..	DD	DC	..	DW	DX	DY	DZ	EA	EB
9	..	..	CA	..	..	CB	..	..	EQ	..	..	EP	..	..	EQ	..	..	ER	..	..	ES	..	..	ET	EU	EV	EW	EX	EY	EZ
10	AE	AF	..	AC	AD	..	CV	..	..	CU	..	..	CY	CZ	..	CW	CX	..	DC	DD	..	DA	DB	..	DH	DI	DJ	DE	DF	DG
11	AF	AE	..	AD	AC	..	..	CV	..	..	CU	..	CZ	CY	..	CX	CW	..	DD	DC	..	DB	DA	..	DZ	EA	EB	DW	DX	DY
12	..	..	CB	..	..	CA	..	..	EP	..	..	EQ	..	..	ER	..	..	EQ	..	..	ET	..	..	ES	EX	EY	EZ	EU	EV	EW
13	AG	AH	..	AI	AJ	..	CW	CX	..	CY	CZ	..	FI	..	..	FJ	..	..	FK	FL	..	FM	FN	..	FQ	FP	FQ	FR	FS	FT
14	AH	AG	..	AJ	AI	..	CX	CW	..	CZ	CY	..	..	FI	..	..	FJ	..	FL	FK	..	FN	FM	..	GG	GH	GI	GJ	GK	GL
15	..	..	CC	..	..	CD	..	..	EQ	..	..	ER	..	..	GY	..	..	GZ	..	..	HA	..	..	HB	HG	HD	HE	HF	HG	HH
16	AI	AJ	..	AG	AH	..	CY	CZ	..	CW	CX	..	FJ	..	..	FI	..	..	FM	FN	..	FK	FL	..	FR	FS	FT	FQ	FP	FQ
17	AJ	AI	..	AH	AG	..	CZ	CY	..	CX	CW	..	..	FJ	..	..	FI	..	FN	FM	..	FL	FK	..	GJ	GK	GL	GG	GH	GI
18	..	..	CD	..	..	CC	..	..	ER	..	..	EQ	..	..	GZ	..	..	GY	..	..	HB	..	..	HA	HF	HG	HH	HC	HD	HE
19	AK	AL	..	AM	AN	..	DA	DB	..	DC	DD	..	FK	FL	..	FM	FN	..	HQ	..	..	HR	..	..	HS	HT	HU	HV	HW	HX
20	AL	AK	..	AN	AM	..	DB	DA	..	DD	DC	..	FL	FK	..	FN	FM	..	..	HQ	..	..	HR	..	IK	IL	IM	IN	IO	IP
21	..	..	CE	..	..	CF	..	..	ES	..	..	ET	..	..	HA	..	..	HB	..	..	JC	..	..	JD	JE	JF	JG	JH	JI	JJ
22	AM	AN	..	AK	AL	..	DC	DD	..	DA	DB	..	FM	FN	..	FK	FL	..	HR	..	..	HQ	..	..	HV	HW	HX	HS	HT	HU
23	AN	AM	..	AL	AK	..	DD	DC	..	DB	DA	..	FN	FM	..	FL	FK	..	..	HR	..	..	HQ	..	IN	IO	IP	IK	IL	IM
24	..	..	CF	..	..	CE	..	..	ET	..	..	ES	..	..	HB	..	..	HA	..	..	JD	..	..	JC	JH	JI	JJ	JE	JF	JG
25	AO	BG	CG	AR	BJ	CJ	DE	DW	EU	DH	DZ	EX	FO	GG	HC	FR	GJ	HF	HS	IK	JE	HV	IN	JH	JS	JT	JU	JV	JW	JX
26	AP	BH	CH	AS	BK	CK	DF	DX	EV	DI	EA	EY	FP	GH	HD	FS	GK	HG	HT	IL	JF	HW	IO	JI	JT	KK	KL	JW	KM	KN
27	AQ	BI	CI	AT	BL	CL	DG	DY	EW	DJ	EB	EZ	FQ	GI	HE	FT	GL	HH	HU	IM	JG	HX	IP	JJ	JU	KL	LA	JX	KN	LB
28	AR	BJ	CJ	AO	BG	CG	DH	DZ	EX	DE	DW	EU	FR	GJ	HF	FO	GG	HC	HV	IN	JH	HS	IK	JE	JV	JW	JX	JS	JT	JU
29	AS	BK	CK	AP	BH	CH	DI	EA	EY	DF	DX	EV	FS	GK	HG	FP	GH	HD	HW	IO	JI	HT	IL	JF	JW	KM	KN	JT	KK	KL
30	AT	BL	CL	AQ	BI	CI	DJ	EB	EZ	DG	DY	EW	FT	GL	HH	FQ	GI	HE	HX	IP	JJ	HU	IM	JG	JX	KN	LB	JU	KL	LA
31	AU	BM	CM	AK	BP	CO	DK	EC	FA	DN	EF	FC	FU	GM	HI	FX	GP	HK	HY	IQ	JK	IB	IT	JM	JY	KO	LC	KB	KR	LF
32	AV	BN	CN	AY	BQ	CP	DL	ED	FB	DO	EG	FD	FV	GN	HJ	FY	GQ	HL	HZ	IR	JL	IC	IU	JN	JZ	KP	LD	KC	KS	LG
33	AW	BO	CI	AZ	BR	CL	DM	EE	EW	DP	EH	EZ	FW	GO	HE	FZ	GR	HH	IA	IS	JG	ID	IV	JJ	KA	KQ	LE	KD	KT	LH
34	AX	BP	CO	AU	BM	CM	DN	EF	FC	DK	EC	FA	FX	GP	HK	FU	GM	HI	IB	IT	JM	HY	IQ	JK	KB	KR	LF	JY	KO	LC
35	AY	BQ	CP	AV	BN	CN	DO	EG	FD	DL	ED	FB	FY	GQ	HL	FV	GN	HJ	IC	IU	JN	HZ	IR	JL	KC	KS	LG	JZ	KP	LD
36	AZ	BR	CL	AW	BO	CI	DP	EH	EZ	DM	EE	EW	FZ	GR	HH	FW	GO	HE	ID	IV	JJ	IA	IS	JG	KD	KT	LH	KA	KQ	LE
37	BA	BS	CQ	BD	BV	CS	DQ	EI	FE	DT	EL	FG	GA	GS	HM	GD	GV	HO	IE	IW	JQ	IH	IZ	JQ	KE	KU	LI	KH	KX	LK
38	BB	BT	CR	BE	BW	CT	DR	EJ	FF	DU	EM	FH	GB	GT	HN	GE	GW	HP	IF	IX	JP	II	JA	JR	KF	KV	LJ	KI	KY	LL
39	BC	BU	CI	BF	BX	CL	DS	EK	EW	DV	EN	EZ	GC	GU	HE	GF	GX	HH	IG	IY	JG	IJ	JB	JJ	KG	KW	LE	KJ	KZ	LH
40	BD	BV	CS	BA	BS	CQ	DT	EL	FG	DQ	EI	FE	GD	GV	HO	GA	GS	HM	IH	IZ	JQ	IE	IW	JO	KH	KX	LK	KE	KU	LI
41	BE	BW	CT	BB	BT	CR	DU	EM	FH	DR	EJ	FF	GE	GW	HP	GB	GT	HN	II	JA	JR	IF	IX	JP	KI	KY	LL	KF	KV	LJ
42	BF	BX	CL	BC	BU	CI	DV	EN	EZ	DS	EK	EW	GF	GX	HH	GC	GU	HE	IJ	JB	JJ	IG	IY	JG	KJ	KZ	LH	KG	KW	LE

PHASE ANGLE MATRIX

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	0	0	0	180	0	0	180	0	0	0	0	0	0	0	0	0	180	0	0	0	0	0	0	0	0	0	180	180	180	180
2	0	0	0	0	180	0	180	180	0	180	0	0	180	0	0	0	0	0	180	0	0	180	0	0	180	180	0	0	0	0
3	0	0	180	0	0	180	0	0	180	0	0	0	0	0	180	0	0	0	0	0	180	0	0	0	180	180	0	0	0	0
4	180	0	0	0	0	0	0	0	0	180	0	0	0	180	0	0	0	0	0	0	0	0	0	0	0	0	0	180	180	180
5	0	180	0	0	0	0	180	0	0	180	180	0	0	0	0	180	0	0	180	0	0	180	0	0	0	0	180	180	180	0
6	0	0	180	0	0	180	0	0	0	0	0	180	0	0	0	0	180	0	0	0	180	0	0	180	0	0	0	180	180	0
7	180	180	0	0	180	0	0	0	0	180	0	0	180	0	0	180	0	0	180	0	0	180	0	0	0	180	0	0	0	180
8	0	180	0	0	0	0	0	0	0	0	180	0	180	180	0	0	0	0	180	0	0	0	0	0	180	180	0	180	180	180
9	0	0	180	0	0	0	0	0	180	0	0	0	0	0	0	180	0	0	180	180	0	180	180	0	0	0	180	180	0	0
10	0	180	0	180	180	0	180	0	0	0	0	0	180	180	0	180	180	0	0	180	0	180	180	0	0	0	0	0	180	0
11	0	0	0	0	180	0	0	180	0	0	0	0	180	180	0	0	0	0	0	0	0	0	0	0	0	0	180	0	0	0
12	0	0	0	0	0	180	0	0	0	0	0	180	0	0	180	0	0	0	0	0	0	0	0	0	180	180	180	180	0	0
13	0	180	0	0	0	0	180	180	0	180	180	0	180	0	0	180	0	0	180	0	0	180	0	0	180	180	0	180	180	180
14	0	0	0	180	0	0	0	180	0	0	180	0	0	180	0	0	180	0	0	180	0	0	0	0	180	0	180	0	180	180
15	0	0	180	0	0	0	0	0	0	180	0	0	0	0	0	0	0	180	0	0	0	0	0	180	180	0	180	180	180	0
16	0	0	0	0	180	0	180	180	0	180	180	0	180	0	0	180	0	0	0	0	0	0	180	0	180	180	0	180	180	180
17	180	0	0	0	0	0	0	180	0	0	180	0	0	180	0	0	180	0	180	0	0	180	0	0	180	0	180	0	0	0
18	0	0	0	0	0	180	0	0	180	0	0	0	0	0	180	0	0	0	0	0	180	0	0	0	0	180	180	180	180	0
19	0	180	0	0	180	0	180	180	0	180	180	0	180	180	0	0	0	0	0	0	0	0	0	0	0	180	180	0	180	180
20	0	0	0	0	0	0	0	180	0	180	180	0	180	180	0	0	0	0	180	0	0	0	0	0	0	180	180	0	0	180
21	0	0	180	0	0	0	0	0	0	0	0	0	0	0	0	0	180	0	0	0	0	0	0	0	0	180	180	180	180	0
22	0	180	0	0	180	0	180	0	0	180	180	0	0	180	0	180	0	0	0	0	0	0	0	0	0	180	180	180	180	180
23	0	0	0	0	0	0	180	180	0	0	180	0	0	0	0	180	0	0	0	0	0	0	0	0	0	180	180	0	0	0
24	0	0	0	0	0	180	0	0	0	0	0	0	0	0	180	0	0	0	0	0	0	0	0	0	180	180	180	180	180	0
25	0	180	0	180	0	180	0	0	180	180	0	0	180	180	0	180	180	0	180	180	180	180	180	180	180	180	180	0	0	180
26	0	180	0	180	0	0	180	180	0	180	180	0	180	180	0	180	0	0	180	0	0	180	180	180	180	180	180	0	0	180
27	180	0	0	0	180	180	0	180	0	180	0	180	180	0	0	180	0	180	180	180	0	180	180	0	180	0	0	180	180	0
28	180	0	0	0	180	180	180	0	180	0	0	0	180	180	0	180	180	180	180	180	0	180	180	0	0	0	180	180	0	0
29	180	0	180	0	180	180	180	0	180	0	180	0	0	180	180	180	180	0	180	180	0	180	180	180	0	0	0	180	180	0
30	180	0	180	0	180	0	0	180	180	180	0	0	180	180	180	180	180	180	180	180	0	180	0	0	0	0	0	180	180	0
31	0	180	180	180	0	0	0	180	0	0	0	180	180	180	180	180	180	180	0	0	180	0	0	0	0	180	180	0	180	0
32	0	0	0	180	180	180	180	180	180	180	180	0	0	0	0	0	180	180	0	180	0	0	0	180	0	0	0	180	0	0
33	0	180	0	180	0	180	180	0	0	180	180	0	0	180	180	0	180	180	180	180	180	180	180	180	0	180	0	0	180	0
34	180	0	180	0	180	0	0	0	0	0	180	180	180	0	180	0	0	180	180	0	180	0	0	0	180	0	0	0	0	0
35	180	180	0	0	0	180	180	180	180	180	180	0	0	180	0	0	0	180	180	0	180	180	0	0	0	180	0	180	180	0
36	0	180	180	180	0	0	0	0	180	0	180	0	180	0	180	180	180	0	180	0	0	180	0	180	180	180	0	0	180	180
37	180	180	0	0	0	0	180	0	0	180	0	0	180	0	180	180	180	0	180	0	0	180	0	180	0	180	180	180	180	180
38	0	0	180	180	180	0	0	0	0	180	0	180	0	180	180	0	180	180	0	0	180	0	0	180	0	0	0	0	0	0
39	0	0	0	180	180	180	180	180	180	0	0	0	180	0	0	0	0	0	180	0	0	180	0	180	180	0	180	180	180	180
40	0	0	180	180	180	180	180	0	180	180	0	180	180	180	180	180	0	0	180	0	0	180	180	180	180	180	0	180	0	0
41	180	180	180	0	0	0	180	0	0	0	0	180	0	180	0	0	180	0	0	180	180	0	180	180	180	180	0	180	180	0
42	0	0	180	180	180	0	180	180	180	0	0	0	180	180	180	180	180	0	0	180	180	180	180	0	180	180	0	0	180	0

AMPLITUDES

	31	32	33	34	35	36	37	38	39	40	41	42
1	AU	AV	AW	AX	AY	AZ	BA	BB	BC	BD	BE	BF
2	BM	BN	BO	BP	BQ	BR	BS	BT	BU	BV	BW	BX
3	CM	CN	CI	CO	CP	CL	CQ	CR	CI	CS	CT	CL
4	AX	AY	AZ	AU	AV	AW	BD	BE	BF	BA	BB	BC
5	BP	BQ	BR	BM	BN	BO	BV	BW	BX	BS	BT	BU
6	CO	CP	CL	CM	CN	CI	CS	CT	CL	CQ	CR	CI
7	DK	DL	DM	DN	DO	DP	DQ	DR	DS	DT	DU	DV
8	EC	ED	EE	EF	EG	EH	EI	EJ	EK	EL	EM	EN
9	FA	FB	EW	FC	FD	EZ	FE	FF	EW	FG	FH	EZ
10	DN	DO	DP	DK	DL	DM	DT	DU	DV	DQ	DR	DS
11	EF	EG	EH	EC	ED	EE	EL	EM	EN	EI	EJ	EK
12	FC	FD	EZ	FA	FB	EW	FG	FH	EZ	FE	FF	EW
13	FU	FV	FW	FX	FY	FZ	GA	GB	GC	GD	GE	GF
14	GM	GN	GO	GP	GQ	GR	GS	GT	GU	GV	GW	GX
15	HI	HJ	HE	HK	HL	HH	HM	HN	HE	HO	HP	HH
16	FX	FY	FZ	FU	FV	FW	GD	GE	GF	GA	GB	GC
17	GP	GQ	GR	GM	GN	GO	GV	GW	GX	GS	GT	GU
18	HK	HL	HH	HI	HJ	HE	HO	HP	HH	HM	HN	HE
19	HY	HZ	IA	IB	IC	ID	IE	IF	IG	IH	II	IJ
20	IQ	IR	IS	IT	IU	IV	IW	IX	IY	IZ	JA	JB
21	JK	JL	JG	JM	JN	JJ	JO	JP	JG	JQ	JR	JJ
22	IB	IC	ID	HY	HZ	IA	IH	II	IJ	IE	IF	IG
23	IT	IU	IV	IQ	IR	IS	IZ	JA	JB	IW	IX	IY
24	JM	JN	JJ	JK	JL	JG	JQ	JR	JJ	JO	JP	JG
25	JY	JZ	KA	KB	KC	KD	KE	KF	KG	KH	KI	KJ
26	KO	KP	KQ	KR	KS	KT	KU	KV	KW	KX	KY	KZ
27	LC	LD	LE	LF	LG	LH	LI	LJ	LE	LK	LL	LH
28	KB	KC	KD	JY	JZ	KA	KH	KI	KJ	KE	KF	KG
29	KR	KS	KT	KO	KP	KQ	KX	KY	KZ	KU	KV	KW
30	LF	LG	LH	LC	LD	LE	LK	LL	LH	LI	LJ	LE
31	LM	LN	LO	LP	LQ	LR	LS	LT	LU	LV	LW	LX
32	LN	LY	LZ	LQ	MA	MB	MC	MD	ME	MF	MG	MH
33	LO	LZ	LA	LR	MB	LB	MI	MJ	LE	MK	ML	LH
34	LP	LQ	LR	LM	LN	LO	LV	LW	LX	LS	LT	LU
35	LQ	MA	MB	LN	LY	LZ	MF	MG	MH	MC	MD	ME
36	LR	MB	LB	LO	LZ	LA	MK	ML	LH	MI	MJ	LE
37	LS	MC	MI	LV	MF	MK	MM	MN	MO	MP	MQ	MR
38	LT	MD	MJ	LW	MG	ML	MN	MS	MT	MQ	MU	MV
39	LU	ME	LE	LX	MH	LH	MO	MT	LA	MR	MV	LB
40	LV	MF	MK	LS	MC	MI	MP	MQ	MR	MM	MN	MO
41	LW	MG	ML	LT	MD	MJ	MQ	MU	MV	MN	MS	MT
42	LX	MH	LH	LU	ME	LE	MR	MV	LB	MO	MT	LA

PHASE ANGLE MATRIX

	31	32	33	34	35	36	37	38	39	40	41	42
1	0	0	0	180	180	0	180	0	0	0	180	0
2	180	0	180	0	180	180	180	0	0	0	180	0
3	180	0	0	180	0	180	0	180	0	180	180	180
4	180	180	180	0	0	180	0	180	180	180	0	180
5	0	180	0	180	0	0	0	180	180	180	0	180
6	0	180	180	0	180	0	0	0	180	180	0	0
7	0	180	180	0	180	0	180	0	180	180	180	180
8	180	180	0	0	180	0	0	0	180	0	0	180
9	0	180	0	0	180	180	0	0	0	180	0	180
10	0	180	180	0	180	0	180	180	0	180	0	0
11	0	180	180	180	180	180	0	0	0	0	0	0
12	180	0	180	180	0	0	0	180	180	180	180	0
13	180	0	0	180	0	180	180	0	0	180	0	180
14	180	0	180	180	180	0	0	180	0	180	180	180
15	180	0	0	0	0	180	180	180	0	180	0	180
16	180	0	0	180	0	180	180	0	0	180	0	180
17	180	180	180	180	0	0	180	180	0	0	180	180
18	180	180	180	0	180	0	0	180	180	0	0	0
19	180	0	0	180	180	180	180	0	0	180	0	0
20	180	0	180	0	0	180	0	180	0	0	180	180
21	0	180	0	180	180	180	0	0	0	0	180	180
22	180	180	0	180	0	180	180	0	180	180	0	180
23	0	0	0	180	0	0	0	180	0	0	180	180
24	0	0	180	180	0	0	180	0	180	180	180	0
25	0	0	0	180	180	0	180	180	180	0	180	180
26	0	0	0	0	0	180	180	0	0	180	180	180
27	0	180	0	180	0	0	0	180	0	0	0	0
28	180	180	180	0	0	180	0	180	0	180	180	0
29	0	0	0	0	0	180	180	180	0	180	0	180
30	0	180	0	180	0	0	180	180	0	180	0	0
31	180	0	0	0	0	0	0	180	180	0	0	180
32	0	0	180	0	180	0	180	180	0	0	180	0
33	0	180	0	180	180	180	0	0	0	0	180	0
34	0	0	180	180	0	180	0	0	0	0	180	0
35	0	180	180	0	0	0	0	180	180	180	180	180
36	0	0	180	180	0	0	180	0	0	180	180	0
37	0	180	0	0	0	180	0	0	180	180	180	180
38	180	180	0	0	180	0	0	180	0	180	0	0
39	180	0	0	0	180	0	180	0	0	0	180	180
40	0	0	0	0	180	180	180	180	0	0	0	0
41	0	180	180	180	180	180	180	0	180	0	180	180
42	180	0	0	0	180	0	180	0	180	0	180	0

SYMMETRY COORDINATES

IR	D	M
1	1	1
0.0	0.0
0.0	0.0
0.70711	0.00000
0.0	0.0
0.0	0.0
0.70711	0.00000
0.0	0.0
0.0	0.0
0.0	0.0

0.40825	0.00000
0.0	0.0
0.17678	-0.30619
0.10206	-0.17678
0.0	0.0
0.17678	-0.30619
0.10206	-0.17678
0.0	0.0
-0.17678	-0.30619
0.10206	0.17678
0.0	0.0
-0.17678	-0.30619
0.10206	0.17678
0.0	0.0

IR	D	M
2	2	5

0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.40825	0.00000
0.0	0.0
0.0	0.0
0.40825	0.00000
0.0	0.0
0.0	0.0
0.10206	0.17678
-0.17678	-0.30619
0.0	0.0
0.10206	0.17678
-0.17678	-0.30619
0.0	0.0
0.10206	-0.17678
0.17678	-0.30619
0.0	0.0
0.10206	-0.17678
0.17678	-0.30619
0.0	0.0

IR	D	M
3	1	4

0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.50000	0.00000
0.00000	-0.50000
0.0	0.0
-0.50000	-0.00000
-0.00000	0.50000
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0

0.0	0.0
-0.40825	-0.00000
0.0	0.0
0.0	0.0
-0.20412	0.35355
0.0	0.0
0.0	0.0
0.20413	-0.35355
0.0	0.0
0.0	0.0
-0.20412	-0.35355
0.0	0.0
0.0	0.0
0.20412	0.35355

IR	D	M
2	2	6

0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
-0.00000	-0.00000
0.40825	0.00000
0.0	0.0
-0.00000	-0.00000
0.40825	0.00000
0.0	0.0
0.17678	0.30619
0.10206	0.17678
0.0	0.0
0.17678	0.30619
0.10206	0.17678
0.0	0.0
-0.17678	0.30619
0.10206	-0.17678
0.0	0.0
-0.17678	0.30619
0.10206	-0.17678
0.0	0.0

IR	D	M
3	1	5

0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0
0.0	0.0

```
   IR  D  M          IR  D  M          IR  D  M          IR  D  M          IR  D  M          IR  D  M
    3  2  3           3  2  4           3  2  5           3  2  6           3  2  7           4  1  1
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.70711   0.00001
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0    -0.70711  -0.00001
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.50000   0.00000 0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
 -0.00000   0.50000 0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
 -0.50000  -0.00000 0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.00000  -0.50000 0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.50000   0.00000 0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0    -0.00000   0.50000 0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0    -0.50000  -0.00000 0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.00000  -0.50000 0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.40825   0.00000 0.00000   0.00000 0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.40825   0.00000 0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.40825   0.00000 0.0       0.0
  0.0       0.0     0.0       0.0    -0.40825  -0.00000 -0.00000  -0.00000 0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0    -0.40825  -0.00000 0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.40825   0.00000 0.0       0.0
  0.0       0.0     0.0       0.0     0.10206  -0.17678 0.17678  -0.30619 0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0    -0.17678   0.30619 0.10206  -0.17678 0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0    -0.20412   0.35355 0.0       0.0
  0.0       0.0     0.0       0.0    -0.10206   0.17678 -0.17678  0.30619 0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.17678  -0.30619 -0.10206  0.17678 0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0    -0.20412   0.35355 0.0       0.0
  0.0       0.0     0.0       0.0     0.10206   0.17678 -0.17678 -0.30619 0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.17678   0.30619 0.10206   0.17678 0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0    -0.20412  -0.35355 0.0       0.0
  0.0       0.0     0.0       0.0    -0.10206  -0.17678 0.17678   0.30619 0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0    -0.17678  -0.30619 -0.10206 -0.17678 0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0    -0.20412  -0.35355 0.0       0.0
   IR  D  M          IR  D  M          IR  D  M          IR  D  M          IR  D  M          IR  D  M
    4  1  2           4  1  3           4  1  4           4  1  5           4  1  6           4  1  7
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.70711   0.00001 0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
 -0.70711  -0.00001 0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.70711   0.00001 0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0    -0.70711  -0.00001 0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.70711   0.00001 0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0    -0.70711  -0.00001 0.0       0.0     0.0       0.0     0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.40825   0.00001 -0.00000  -0.00000 0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.40825   0.00001 0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.40825   0.00001
  0.0       0.0     0.0       0.0     0.0       0.0     0.40825   0.00000 -0.00000  -0.00000 0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.40825   0.00000 0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0    -0.40825  -0.00000
  0.0       0.0     0.0       0.0     0.0       0.0    -0.20412  -0.00000 -0.35355  -0.00000 0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.35355   0.00000 -0.20412  -0.00000 0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.40825   0.00000
  0.0       0.0     0.0       0.0     0.0       0.0    -0.20412  -0.00000 -0.35355  -0.00000 0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.35355   0.00000 -0.20412  -0.00000 0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0    -0.40825  -0.00001
  0.0       0.0     0.0       0.0     0.0       0.0    -0.20412  -0.00000 0.35355   0.00000 0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0    -0.35355  -0.00000 -0.20412  -0.00000 0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.40825   0.00000
  0.0       0.0     0.0       0.0     0.0       0.0    -0.20412  -0.00000 0.35355   0.00000 0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0    -0.35355  -0.00000 -0.20412  -0.00000 0.0       0.0
  0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0     0.0       0.0    -0.40825  -0.00000
```

ELEMENTS OF THE BLOCK-DIAGONALIZED DYNAMICAL MATRIX

IR NUMBER 1 IS INFRARED ACTIVE.
IR NUMBER 1 IS RAMAN ACTIVE.
IR NUMBER 2 IS INFRARED ACTIVE.
IR NUMBER 2 IS RAMAN ACTIVE.
IR NUMBER 3 IS RAMAN ACTIVE.

GROUP THEORETICAL ANALYSIS OF THE K LI SO4-STRUCTURE
0 0 1 -DIRECTION

CHARACTER TABLE

```
OP    IR( 1)     IR( 2)     IR( 3)     IR( 4)     IR( 5)     IR( 6)
 1    1.0 -0.0   1.0 -0.0   1.0 -0.0   1.0 -0.0   1.0 -0.0   1.0 -0.0
 2    1.0 -0.0   0.5 -0.9  -0.5 -0.9  -1.0  0.0  -0.5  0.9   0.5  0.9
 3    1.0 -0.0  -0.5 -0.9  -0.5  0.9   1.0 -0.0  -0.5 -0.9  -0.5  0.9
 4    1.0 -0.0  -1.0  0.0   1.0 -0.0  -1.0  0.0   1.0 -0.0  -1.0  0.0
 5    1.0 -0.0  -0.5  0.9  -0.5 -0.9   1.0 -0.0  -0.5  0.9  -0.5 -0.9
 6    1.0 -0.0   0.5  0.9  -0.5  0.9  -1.0  0.0  -0.5 -0.9   0.5 -0.9
```

TABLE OF PHASES AND CHARACTERS FOR THE T MATRICES.

THE CHARACTER OF T(R(1)) IS (42.00000, 0.0)

THE CHARACTER OF T(R(2)) IS (0.0 , 0.0)

THE CHARACTER OF T(R(3)) IS (0.0 , 0.0)

A.2 IND

OUTPUT

```
THERE ARE  5 DIFFERENT UNIT TYPES
    NAMELY :
             UNIT  1 = K1
             UNIT  3 = LI1
             UNIT  5 = S1
             UNIT  7 = O1
             UNIT  9 = O2

A MAXIMUM OF  32 INTERACTIONS CAN BE SPECIFIED
    NAMELY :
             INTERACTION   1 BETWEEN  K1   AND K1
             INTERACTION   2 BETWEEN  K1   AND K2
             INTERACTION   3 BETWEEN  K1   AND LI1
             INTERACTION   4 BETWEEN  K1   AND LI2
             INTERACTION   5 BETWEEN  K1   AND S1
             INTERACTION   6 BETWEEN  K1   AND S2
             INTERACTION   7 BETWEEN  K1   AND O1
             INTERACTION   8 BETWEEN  K1   AND O5
             INTERACTION   9 BETWEEN  K1   AND O2
             INTERACTION  10 BETWEEN  K1   AND O6
             INTERACTION  11 BETWEEN  LI1  AND LI1
             INTERACTION  12 BETWEEN  LI1  AND LI2
             INTERACTION  13 BETWEEN  LI1  AND S1
             INTERACTION  14 BETWEEN  LI1  AND S2
             INTERACTION  15 BETWEEN  LI1  AND O1
             INTERACTION  16 BETWEEN  LI1  AND O5
             INTERACTION  17 BETWEEN  LI1  AND O2
             INTERACTION  18 BETWEEN  LI1  AND O6
             INTERACTION  19 BETWEEN  S1   AND S1
             INTERACTION  20 BETWEEN  S1   AND S2
             INTERACTION  21 BETWEEN  S1   AND O1
             INTERACTION  22 BETWEEN  S1   AND O5
             INTERACTION  23 BETWEEN  S1   AND O2
             INTERACTION  24 BETWEEN  S1   AND O6
             INTERACTION  25 BETWEEN  O1   AND O1
             INTERACTION  26 BETWEEN  O1   AND O5
             INTERACTION  27 BETWEEN  O1   AND O2
             INTERACTION  28 BETWEEN  O1   AND O6
             INTERACTION  29 BETWEEN  O2   AND O2
             INTERACTION  30 BETWEEN  O2   AND O6
             INTERACTION  31 BETWEEN  O2   AND O3
             INTERACTION  32 BETWEEN  O2   AND O7
```

A.3 NN

INPUT

```
     1     2     0
    10
  .005       15.00
```

OUTPUT

```
K1   HAS  6 NEIGHBORS OF TYPE K1   AT THE DISTANCE  5.14 A IN THE CELLS :      WITH RADIUS VECTOR :
(-1 -1  0)                                                                  ( -2.571 -4.453  0.0  )
(-1  0  0)                                                                  ( -5.142  0.0    0.0  )
( 0 -1  0)                                                                  (  2.571 -4.453  0.0  )
( 0  1  0)                                                                  ( -2.571  4.453  0.0  )
( 1  0  0)                                                                  (  5.142  0.0    0.0  )
( 1  1  0)                                                                  (  2.571  4.453  0.0  )

K1   HAS  2 NEIGHBORS OF TYPE K1   AT THE DISTANCE  8.62 A IN THE CELLS :      WITH RADIUS VECTOR :
( 0  0 -1)                                                                  (  0.0    0.0   -8.624)
( 0  0  1)                                                                  (  0.0    0.0    8.624)

K1   HAS  6 NEIGHBORS OF TYPE K1   AT THE DISTANCE  8.91 A IN THE CELLS :      WITH RADIUS VECTOR :
(-2 -1  0)                                                                  ( -7.713 -4.453  0.0  )
(-1 -2  0)                                                                  (  0.0   -8.906  0.0  )
(-1  1  0)                                                                  ( -7.713  4.453  0.0  )
( 1 -1  0)                                                                  (  7.713 -4.453  0.0  )
( 1  2  0)                                                                  (  0.0    8.906  0.0  )
( 2  1  0)                                                                  (  7.713  4.453  0.0  )

K1   HAS 12 NEIGHBORS OF TYPE K1   AT THE DISTANCE 10.04 A IN THE CELLS :      WITH RADIUS VECTOR :
(-1 -1 -1)                                                                  ( -2.571 -4.453 -8.624)
(-1 -1  1)                                                                  ( -2.571 -4.453  8.624)
(-1  0 -1)                                                                  ( -5.142  0.0   -8.624)
(-1  0  1)                                                                  ( -5.142  0.0    8.624)
( 0 -1 -1)                                                                  (  2.571 -4.453 -8.624)
( 0 -1  1)                                                                  (  2.571 -4.453  8.624)
( 0  1 -1)                                                                  ( -2.571  4.453 -8.624)
( 0  1  1)                                                                  ( -2.571  4.453  8.624)
( 1  0 -1)                                                                  (  5.142  0.0   -8.624)
( 1  0  1)                                                                  (  5.142  0.0    8.624)
( 1  1 -1)                                                                  (  2.571  4.453 -8.624)
( 1  1  1)                                                                  (  2.571  4.453  8.624)

K1   HAS  6 NEIGHBORS OF TYPE K1   AT THE DISTANCE 10.28 A IN THE CELLS :      WITH RADIUS VECTOR :
(-2 -2  0)                                                                  ( -5.142 -8.906  0.0  )
(-2  0  0)                                                                  (-10.284  0.0    0.0  )
( 0 -2  0)                                                                  (  5.142 -8.906  0.0  )
( 0  2  0)                                                                  ( -5.142  8.906  0.0  )
( 2  0  0)                                                                  ( 10.284  0.0    0.0  )
( 2  2  0)                                                                  (  5.142  8.906  0.0  )

K1   HAS 12 NEIGHBORS OF TYPE K1   AT THE DISTANCE 12.40 A IN THE CELLS :      WITH RADIUS VECTOR :
(-2 -1 -1)                                                                  ( -7.713 -4.453 -8.624)
(-2 -1  1)                                                                  ( -7.713 -4.453  8.624)
(-1 -2 -1)                                                                  (  0.0   -8.906 -8.624)
(-1 -2  1)                                                                  (  0.0   -8.906  8.624)
(-1  1 -1)                                                                  ( -7.713  4.453 -8.624)
(-1  1  1)                                                                  ( -7.713  4.453  8.624)
( 1 -1 -1)                                                                  (  7.713 -4.453 -8.624)
( 1 -1  1)                                                                  (  7.713 -4.453  8.624)
( 1  2 -1)                                                                  (  0.0    8.906 -8.624)
( 1  2  1)                                                                  (  0.0    8.906  8.624)
( 2  1 -1)                                                                  (  7.713  4.453 -8.624)
( 2  1  1)                                                                  (  7.713  4.453  8.624)
```

```
K1   HAS 12 NEIGHBORS OF TYPE K1   AT THE DISTANCE 13.42 A IN THE CELLS :        WITH RADIUS VECTOR :
                                   (-2 -2 -1)                                  ( -5.142 -8.906 -8.624)
                                   (-2 -2  1)                                  ( -5.142 -8.906  8.624)
                                   (-2  0 -1)                                  (-10.284  0.0   -8.624)
                                   (-2  0  1)                                  (-10.284  0.0    8.624)
                                   ( 0 -2 -1)                                  (  5.142 -8.906 -8.624)
                                   ( 0 -2  1)                                  (  5.142 -8.906  8.624)
                                   ( 0  2 -1)                                  ( -5.142  8.906 -8.624)
                                   ( 0  2  1)                                  ( -5.142  8.906  8.624)
                                   ( 2  0 -1)                                  ( 10.284  0.0   -8.624)
                                   ( 2  0  1)                                  ( 10.284  0.0    8.624)
                                   ( 2  2 -1)                                  (  5.142  8.906 -8.624)
                                   ( 2  2  1)                                  (  5.142  8.906  8.624)

K1   HAS 12 NEIGHBORS OF TYPE K1   AT THE DISTANCE 13.60 A IN THE CELLS :        WITH RADIUS VECTOR :
                                   (-3 -2  0)                                  (-10.284 -8.906  0.0  )
                                   (-3 -1  0)                                  (-12.855 -4.453  0.0  )
                                   (-2 -3  0)                                  ( -2.571-13.359  0.0  )
                                   (-2  1  0)                                  (-12.855  4.453  0.0  )
                                   (-1 -3  0)                                  (  2.571-13.359  0.0  )
                                   (-1  2  0)                                  (-10.284  8.906  0.0  )
                                   ( 1 -2  0)                                  ( 10.284 -8.906  0.0  )
                                   ( 1  3  0)                                  ( -2.571 13.359  0.0  )
                                   ( 2 -1  0)                                  ( 12.855 -4.453  0.0  )
                                   ( 2  3  0)                                  (  2.571 13.359  0.0  )
                                   ( 3  1  0)                                  ( 12.855  4.453  0.0  )
                                   ( 3  2  0)                                  ( 10.284  8.906  0.0  )

K1   HAS  6 NEIGHBORS OF TYPE K1   AT THE DISTANCE 15.43 A IN THE CELLS :        WITH RADIUS VECTOR :
                                   (-3 -3  0)                                  ( -7.713-13.359  0.0  )
                                   (-3  0  0)                                  (-15.426  0.0    0.0  )
                                   ( 0 -3  0)                                  (  7.713-13.359  0.0  )
                                   ( 0  3  0)                                  ( -7.713 13.359  0.0  )
                                   ( 3  0  0)                                  ( 15.426  0.0    0.0  )
                                   ( 3  3  0)                                  (  7.713 13.359  0.0  )

K1   HAS 24 NEIGHBORS OF TYPE K1   AT THE DISTANCE 16.11 A IN THE CELLS :        WITH RADIUS VECTOR :
                                   (-3 -2 -1)                                  (-10.284 -8.906 -8.624)
                                   (-3 -2  1)                                  (-10.284 -8.906  8.624)
                                   (-3 -1 -1)                                  (-12.855 -4.453 -8.624)
                                   (-3 -1  1)                                  (-12.855 -4.453  8.624)
                                   (-2 -3 -1)                                  ( -2.571-13.359 -8.624)
                                   (-2 -3  1)                                  ( -2.571-13.359  8.624)
                                   (-2  1 -1)                                  (-12.855  4.453 -8.624)
                                   (-2  1  1)                                  (-12.855  4.453  8.624)
                                   (-1 -3 -1)                                  (  2.571-13.359 -8.624)
                                   (-1 -3  1)                                  (  2.571-13.359  8.624)
                                   (-1  2 -1)                                  (-10.284  8.906 -8.624)
                                   (-1  2  1)                                  (-10.284  8.906  8.624)
                                   ( 1 -2 -1)                                  ( 10.284 -8.906 -8.624)
                                   ( 1 -2  1)                                  ( 10.284 -8.906  8.624)
                                   ( 1  3 -1)                                  ( -2.571 13.359 -8.624)
                                   ( 1  3  1)                                  ( -2.571 13.359  8.624)
                                   ( 2 -1 -1)                                  ( 12.855 -4.453 -8.624)
                                   ( 2 -1  1)                                  ( 12.855 -4.453  8.624)
                                   ( 2  3 -1)                                  (  2.571 13.359 -8.624)
                                   ( 2  3  1)                                  (  2.571 13.359  8.624)
                                   ( 3  1 -1)                                  ( 12.855  4.453 -8.624)
                                   ( 3  1  1)                                  ( 12.855  4.453  8.624)
                                   ( 3  2 -1)                                  ( 10.284  8.906 -8.624)
                                   ( 3  2  1)                                  ( 10.284  8.906  8.624)

K1   HAS  2 NEIGHBORS OF TYPE K2   AT THE DISTANCE  4.31 A IN THE CELLS :        WITH RADIUS VECTOR :
                                   ( 0  0  0)                                  (  0.0    0.0   -4.312)
                                   ( 0  0  1)                                  (  0.0    0.0    4.312)

K1   HAS 12 NEIGHBORS OF TYPE K2   AT THE DISTANCE  6.71 A IN THE CELLS :        WITH RADIUS VECTOR :
                                   (-1 -1  0)                                  ( -2.571 -4.453 -4.312)
                                   (-1 -1  1)                                  ( -2.571 -4.453  4.312)
                                   (-1  0  0)                                  ( -5.142  0.0   -4.312)
                                   (-1  0  1)                                  ( -5.142  0.0    4.312)
                                   ( 0 -1  0)                                  (  2.571 -4.453 -4.312)
                                   ( 0 -1  1)                                  (  2.571 -4.453  4.312)
                                   ( 0  1  0)                                  ( -2.571  4.453 -4.312)
                                   ( 0  1  1)                                  ( -2.571  4.453  4.312)
                                   ( 1  0  0)                                  (  5.142  0.0   -4.312)
                                   ( 1  0  1)                                  (  5.142  0.0    4.312)
                                   ( 1  1  0)                                  (  2.571  4.453 -4.312)
                                   ( 1  1  1)                                  (  2.571  4.453  4.312)

K1   HAS 12 NEIGHBORS OF TYPE K2   AT THE DISTANCE  9.90 A IN THE CELLS :        WITH RADIUS VECTOR :
                                   (-2 -1  0)                                  ( -7.713 -4.453 -4.312)
                                   (-2 -1  1)                                  ( -7.713 -4.453  4.312)
                                   (-1 -2  0)                                  (  0.0   -8.906 -4.312)
                                   (-1 -2  1)                                  (  0.0   -8.906  4.312)
                                   (-1  1  0)                                  ( -7.713  4.453 -4.312)
                                   (-1  1  1)                                  ( -7.713  4.453  4.312)
                                   ( 1 -1  0)                                  (  7.713 -4.453 -4.312)
                                   ( 1 -1  1)                                  (  7.713 -4.453  4.312)
                                   ( 1  2  0)                                  (  0.0    8.906 -4.312)
                                   ( 1  2  1)                                  (  0.0    8.906  4.312)
                                   ( 2  1  0)                                  (  7.713  4.453 -4.312)
                                   ( 2  1  1)                                  (  7.713  4.453  4.312)

K1   HAS 12 NEIGHBORS OF TYPE K2   AT THE DISTANCE 11.15 A IN THE CELLS :        WITH RADIUS VECTOR :
                                   (-2 -2  0)                                  ( -5.142 -8.906 -4.312)
                                   (-2 -2  1)                                  ( -5.142 -8.906  4.312)
                                   (-2  0  0)                                  (-10.284  0.0   -4.312)
                                   (-2  0  1)                                  (-10.284  0.0    4.312)
                                   ( 0 -2  0)                                  (  5.142 -8.906 -4.312)
                                   ( 0 -2  1)                                  (  5.142 -8.906  4.312)
                                   ( 0  2  0)                                  ( -5.142  8.906 -4.312)
                                   ( 0  2  1)                                  ( -5.142  8.906  4.312)
                                   ( 2  0  0)                                  ( 10.284  0.0   -4.312)
                                   ( 2  0  1)                                  ( 10.284  0.0    4.312)
                                   ( 2  2  0)                                  (  5.142  8.906 -4.312)
                                   ( 2  2  1)                                  (  5.142  8.906  4.312)
```

```
K1   HAS  2 NEIGHBORS OF TYPE K2   AT THE DISTANCE 12.94 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                                ( 0  0 -1)                    (  0.0    0.0  -12.936)
                                                                ( 0  0  2)                    (  0.0    0.0   12.936)

K1   HAS 12 NEIGHBORS OF TYPE K2   AT THE DISTANCE 13.92 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                                (-1 -1 -1)                    ( -2.571 -4.453-12.936)
                                                                (-1 -1  2)                    ( -2.571 -4.453 12.936)
                                                                (-1  0 -1)                    ( -5.142  0.0   -12.936)
                                                                (-1  0  2)                    ( -5.142  0.0    12.936)
                                                                ( 0 -1 -1)                    (  2.571 -4.453-12.936)
                                                                ( 0 -1  2)                    (  2.571 -4.453 12.936)
                                                                ( 0  1 -1)                    ( -2.571  4.453-12.936)
                                                                ( 0  1  2)                    ( -2.571  4.453 12.936)
                                                                ( 1  0 -1)                    (  5.142  0.0   -12.936)
                                                                ( 1  0  2)                    (  5.142  0.0    12.936)
                                                                ( 1  1 -1)                    (  2.571  4.453-12.936)
                                                                ( 1  1  2)                    (  2.571  4.453 12.936)

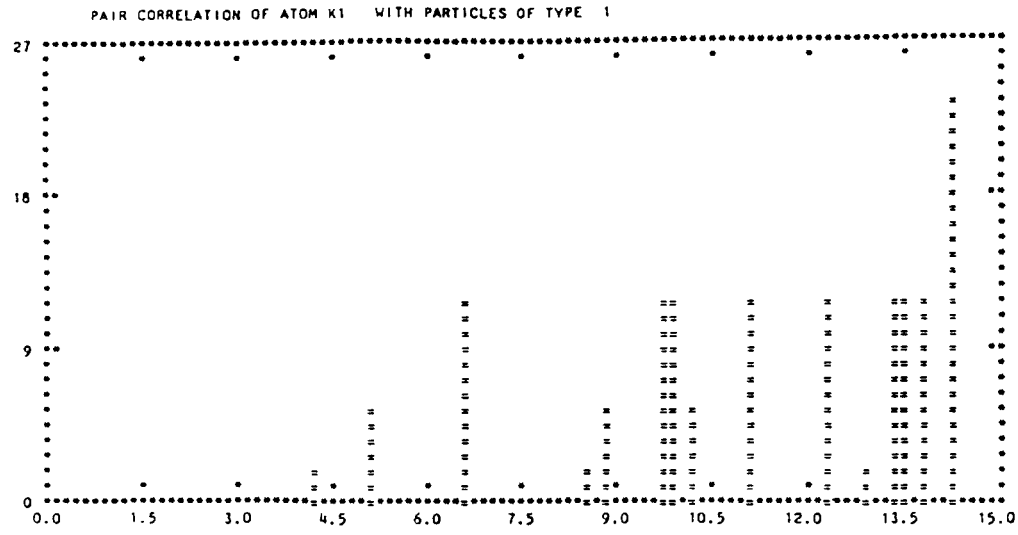
K1   HAS 24 NEIGHBORS OF TYPE K2   AT THE DISTANCE 14.27 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                                (-3 -2  0)                    (-10.284 -8.906 -4.312)
                                                                (-3 -2  1)                    (-10.284 -8.906  4.312)
                                                                (-3 -1  0)                    (-12.855 -4.453 -4.312)
                                                                (-3 -1  1)                    (-12.855 -4.453  4.312)
                                                                (-2 -3  0)                    ( -2.571-13.359 -4.312)
                                                                (-2 -3  1)                    ( -2.571-13.359  4.312)
                                                                (-2  1  0)                    (-12.855  4.453 -4.312)
                                                                (-2  1  1)                    (-12.855  4.453  4.312)
                                                                (-1 -3  0)                    (  2.571-13.359 -4.312)
                                                                (-1 -3  1)                    (  2.571-13.359  4.312)
                                                                (-1  2  0)                    (-10.284  8.906 -4.312)
                                                                (-1  2  1)                    (-10.284  8.906  4.312)
                                                                ( 1 -2  0)                    ( 10.284 -8.906 -4.312)
                                                                ( 1 -2  1)                    ( 10.284 -8.906  4.312)
                                                                ( 1  3  0)                    ( -2.571 13.359 -4.312)
                                                                ( 1  3  1)                    ( -2.571 13.359  4.312)
                                                                ( 2 -1  0)                    ( 12.855 -4.453 -4.312)
                                                                ( 2 -1  1)                    ( 12.855 -4.453  4.312)
                                                                ( 2  3  0)                    (  2.571 13.359 -4.312)
                                                                ( 2  3  1)                    (  2.571 13.359  4.312)
                                                                ( 3  1  0)                    ( 12.855  4.453 -4.312)
                                                                ( 3  1  1)                    ( 12.855  4.453  4.312)
                                                                ( 3  2  0)                    ( 10.284  8.906 -4.312)
                                                                ( 3  2  1)                    ( 10.284  8.906  4.312)

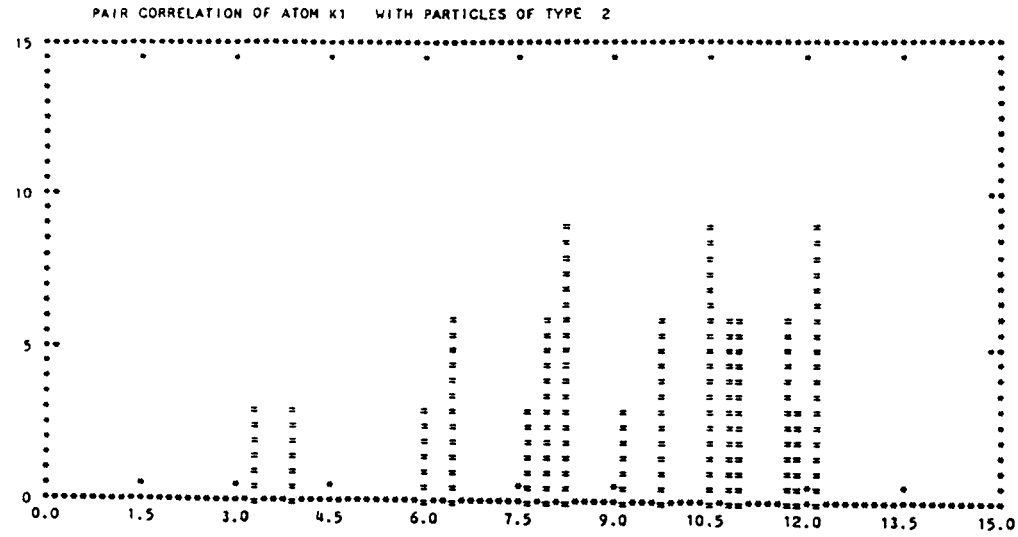
K1   HAS 12 NEIGHBORS OF TYPE K2   AT THE DISTANCE 15.71 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                                (-2 -1 -1)                    ( -7.713 -4.453-12.936)
                                                                (-2 -1  2)                    ( -7.713 -4.453 12.936)
                                                                (-1 -2 -1)                    (  0.0   -8.906-12.936)
                                                                (-1 -2  2)                    (  0.0   -8.906 12.936)
                                                                (-1  1 -1)                    ( -7.713  4.453-12.936)
                                                                (-1  1  2)                    ( -7.713  4.453 12.936)
                                                                ( 1 -1 -1)                    (  7.713 -4.453-12.936)
                                                                ( 1 -1  2)                    (  7.713 -4.453 12.936)
                                                                ( 1  2 -1)                    (  0.0    8.906-12.936)
                                                                ( 1  2  2)                    (  0.0    8.906 12.936)
                                                                ( 2  1 -1)                    (  7.713  4.453-12.936)
                                                                ( 2  1  2)                    (  7.713  4.453 12.936)

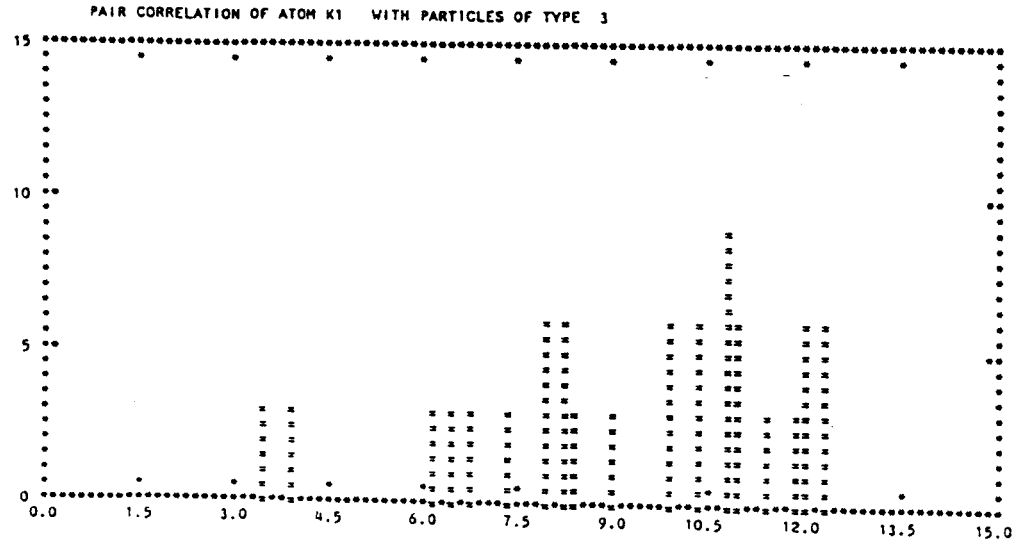
K1   HAS 12 NEIGHBORS OF TYPE K2   AT THE DISTANCE 16.02 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                                (-3 -3  0)                    ( -7.713-13.359 -4.312)
                                                                (-3 -3  1)                    ( -7.713-13.359  4.312)
                                                                (-3  0  0)                    (-15.426  0.0   -4.312)
                                                                (-3  0  1)                    (-15.426  0.0    4.312)
                                                                ( 0 -3  0)                    (  7.713-13.359 -4.312)
                                                                ( 0 -3  1)                    (  7.713-13.359  4.312)
                                                                ( 0  3  0)                    ( -7.713 13.359 -4.312)
                                                                ( 0  3  1)                    ( -7.713 13.359  4.312)
                                                                ( 3  0  0)                    ( 15.426  0.0   -4.312)
                                                                ( 3  0  1)                    ( 15.426  0.0    4.312)
                                                                ( 3  3  0)                    (  7.713 13.359 -4.312)
                                                                ( 3  3  1)                    (  7.713 13.359  4.312)

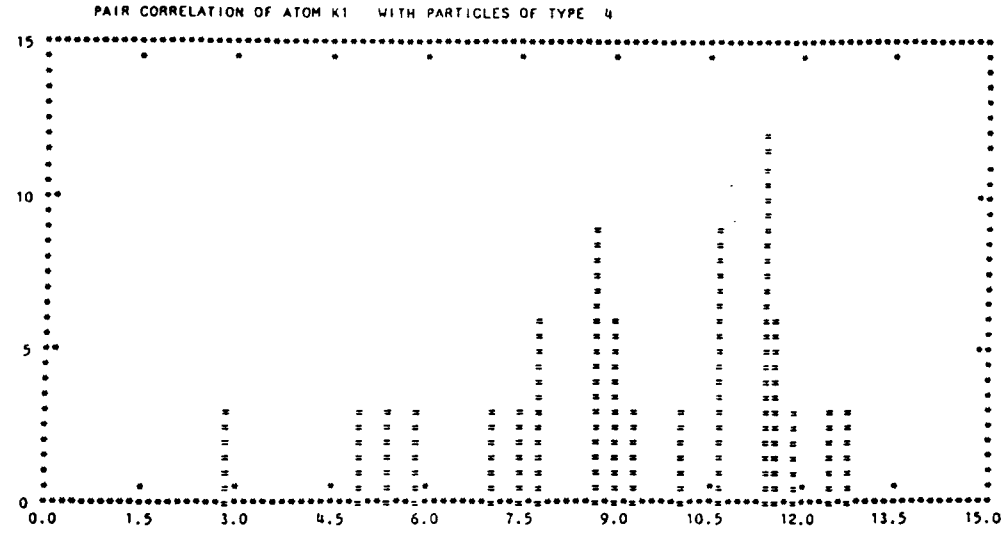
K1   HAS 12 NEIGHBORS OF TYPE K2   AT THE DISTANCE 16.53 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                                (-2 -2 -1)                    ( -5.142 -8.906-12.936)
                                                                (-2 -2  2)                    ( -5.142 -8.906 12.936)
                                                                (-2  0 -1)                    (-10.284  0.0   -12.936)
                                                                (-2  0  2)                    (-10.284  0.0    12.936)
                                                                ( 0 -2 -1)                    (  5.142 -8.906-12.936)
                                                                ( 0 -2  2)                    (  5.142 -8.906 12.936)
                                                                ( 0  2 -1)                    ( -5.142  8.906-12.936)
                                                                ( 0  2  2)                    ( -5.142  8.906 12.936)
                                                                ( 2  0 -1)                    ( 10.284  0.0   -12.936)
                                                                ( 2  0  2)                    ( 10.284  0.0    12.936)
                                                                ( 2  2 -1)                    (  5.142  8.906-12.936)
                                                                ( 2  2  2)                    (  5.142  8.906 12.936)

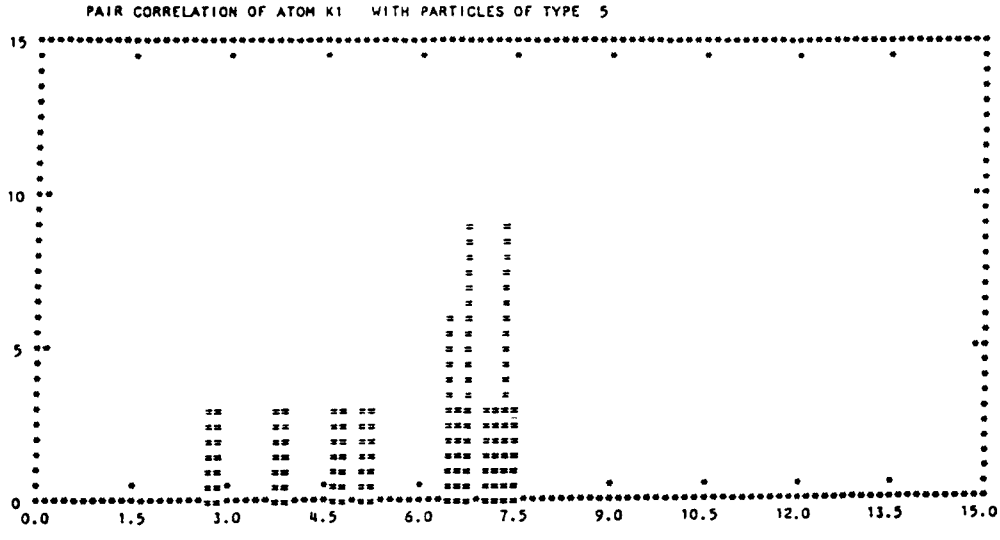
K1   HAS  3 NEIGHBORS OF TYPE LI1  AT THE DISTANCE  4.04 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                                ( 0  0  1)                    (  0.0   -2.969  2.742)
                                                                ( 0  1  1)                    ( -2.571  1.484  2.742)
                                                                ( 1  1  1)                    (  2.571  1.484  2.742)
```


PAIR CORRELATION OF ATOM K1 WITH PARTICLES OF TYPE 1
27
18
9
0
0.0
1.5
3.0
4.5
6.0
7.5
9.0
10.5
12.0
13.5
15.0


PAIR CORRELATION OF ATOM K1 WITH PARTICLES OF TYPE 2
15
10
5
0
0.0
1.5
3.0
4.5
6.0
7.5
9.0
10.5
12.0
13.5
15.0


PAIR CORRELATION OF ATOM K1 WITH PARTICLES OF TYPE 3
15
10
5
0
0.0
1.5
3.0
4.5
6.0
7.5
9.0
10.5
12.0
13.5
15.0


PAIR CORRELATION OF ATOM K1 WITH PARTICLES OF TYPE 4
15
10
5
0
0.0
1.5
3.0
4.5
6.0
7.5
9.0
10.5
12.0
13.5
15.0


PAIR CORRELATION OF ATOM K1 WITH PARTICLES OF TYPE 5
15
10
5
0
0.0
1.5
3.0
4.5
6.0
7.5
9.0
10.5
12.0
13.5
15.0

A.4 MODEL1

INPUT

```
    0     0     0     0     0     1     0     0     0     1
39.10      6.940      32.06      16.00      16.00
    1
    5     7     1
   15    16
    5     9     1
   17    18
    7     9     1
   11    12
    9    11     1
   13    14
    0
    2
    6     7     7     8     9    10
    1     8     1
    1     9     1
    1    10     1
    3     7     1
    3    10     1
    0
    5
     7.
    1     2     3     4     5
    0
1.20       0.40       1.35       -0.850     -0.70      0.1970     0.086      0.106
0.100      2000.      250.0      -.5000     250.       -.30000    700.0      -53.80
700.       -38.6
```

OUTPUT

```
LATTICE DYNAMICAL MODEL-CALCULATION FOR THE FOLLOWING STRUCTURE:

 POSITION VECTOR SPACE LATTICE VECTORS
A 1 = (  5.14200,  0.0     ,  0.0     )
A 2 = ( -2.57100,  4.45300,  0.0     )
A 3 = (  0.0     ,  0.0     ,  8.62400)

AI 1 = (  0.19448,  0.11228,  0.0     )
AI 2 = (  0.0     ,  0.22457,  0.0     )
AI 3 = (  0.0     ,  0.0     ,  0.11595)
 RECIPROCAL SPACE LATTICE VECTORS

      14 PARTICLES PER UNIT CELL :

                              POSITION                          MASS

      K1        (  0.0     ,  0.0     ,  0.0     )      39.10
      K2        (  0.0     ,  0.0     ,  4.31200)      39.10
      LI1       (  0.0     ,  2.96874,  5.88200)       6.94
      LI2       (  2.57100,  1.48437,  1.57000)       6.94
      S1        (  0.0     ,  2.96874,  2.53500)      32.06
      S2        (  2.57100,  1.48437,  6.84700)      32.06
      O1        (  0.0     ,  2.96870,  1.96700)      16.00
      O5        (  2.57100,  1.48440,  8.27900)      16.00
      O2        (  1.39090,  2.92570,  2.06110)      16.00
      O6        (  1.18010,  1.52740,  6.37310)      16.00
      O3        (  4.48380,  4.19480,  2.06110)      16.00
      O7        (  3.22920,  0.25830,  6.37310)      16.00
      O4        (  4.40930,  1.78570,  2.06110)      16.00
      O8        (  3.30370,  2.66740,  6.37310)      16.00
```

MODEL SPECIFICATIONS :

INTERACTION	TYPE	NEIGHBOR	PARAMETER-NO.S								
K1 - K1	COULOMB (M-M)	**	Z1	=	1	Z2	=	1			
K1 - K2	COULOMB (M-M)	**	Z1	=	1	Z2	=	1			
K1 - L11	COULOMB (M-M)	**	Z1	=	1	Z2	=	2			
K1 - L12	COULOMB (M-M)	**	Z1	=	1	Z2	=	2			
K1 - S1	COULOMB (M-M)	**	Z1	=	1	Z2	=	3			
K1 - S2	COULOMB (M-M)	**	Z1	=	1	Z2	=	3			
K1 - O1	COULOMB (M-M)	**	Z1	=	1	Z2	=	4			
K1 - O5	BORN-MAYER	1	R1	=	6	R2	=	8	V0	=	10
	COULOMB (M-M)	**	Z1	=	1	Z2	=	4			
K1 - O2	BORN-MAYER	1	R1	=	6	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5			
K1 - O6	BORN-MAYER	1	R1	=	6	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5			
K1 - O3	BORN-MAYER	1	R1	=	6	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5			
K1 - O7	BORN-MAYER	1	R1	=	6	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5			
K1 - O4	BORN-MAYER	1	R1	=	6	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5			
K1 - O8	BORN-MAYER	1	R1	=	6	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5			
K2 - K2	COULOMB (M-M)	**	Z1	=	1	Z2	=	1			
K2 - L11	COULOMB (M-M)	**	Z1	=	1	Z2	=	2			
K2 - L12	COULOMB (M-M)	**	Z1	=	1	Z2	=	2			
K2 - S1	COULOMB (M-M)	**	Z1	=	1	Z2	=	3			
K2 - S2	COULOMB (M-M)	**	Z1	=	1	Z2	=	3			
K2 - O1	BORN-MAYER	1	R1	=	6	R2	=	8	V0	=	10
	COULOMB (M-M)	**	Z1	=	1	Z2	=	4			
K2 - O5	COULOMB (M-M)	**	Z1	=	1	Z2	=	4			
K2 - O2	BORN-MAYER	1	R1	=	6	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5			
K2 - O6	BORN-MAYER	1	R1	=	6	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5			
K2 - O3	BORN-MAYER	1	R1	=	6	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5			
K2 - O7	BORN-MAYER	1	R1	=	6	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5			
K2 - O4	BORN-MAYER	1	R1	=	6	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5			
K2 - O8	BORN-MAYER	1	R1	=	6	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5			
L11 - L11	COULOMB (M-M)	**	Z1	=	2	Z2	=	2			
L11 - L12	COULOMB (M-M)	**	Z1	=	2	Z2	=	2			
L11 - S1	COULOMB (M-M)	**	Z1	=	2	Z2	=	3			
L11 - S2	COULOMB (M-M)	**	Z1	=	2	Z2	=	3			
L11 - O1	BORN-MAYER	1	R1	=	7	R2	=	8	V0	=	10
	COULOMB (M-M)	**	Z1	=	2	Z2	=	4			
L11 - O5	COULOMB (M-M)	**	Z1	=	2	Z2	=	4			
L11 - O2	COULOMB (M-M)	**	Z1	=	2	Z2	=	5			
L11 - O6	BORN-MAYER	1	R1	=	7	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	2	Z2	=	5			
L11 - O3	COULOMB (M-M)	**	Z1	=	2	Z2	=	5			
L11 - O7	BORN-MAYER	1	R1	=	7	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	2	Z2	=	5			
L11 - O4	COULOMB (M-M)	**	Z1	=	2	Z2	=	5			

LI1 - 08	BORN-MAYER	1	R1	=	7	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	2	Z2	=	5			
LI2 - LI2	COULOMB (M-M)	**	Z1	=	2	Z2	=	2			
LI2 - S1	COULOMB (M-M)	**	Z1	=	2	Z2	=	3			
LI2 - S2	COULOMB (M-M)	**	Z1	=	2	Z2	=	3			
LI2 - 01	COULOMB (M-M)	**	Z1	=	2	Z2	=	4			
LI2 - 05	BORN-MAYER	1	R1	=	7	R2	=	8	V0	=	10
	COULOMB (M-M)	**	Z1	=	2	Z2	=	4			
LI2 - 02	BORN-MAYER	1	R1	=	7	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	2	Z2	=	5			
LI2 - 06	COULOMB (M-M)	**	Z1	=	2	Z2	=	5			
LI2 - 03	BORN-MAYER	1	R1	=	7	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	2	Z2	=	5			
LI2 - 07	COULOMB (M-M)	**	Z1	=	2	Z2	=	5			
LI2 - 04	BORN-MAYER	1	R1	=	7	R2	=	9	V0	=	10
	COULOMB (M-M)	**	Z1	=	2	Z2	=	5			
LI2 - 08	COULOMB (M-M)	**	Z1	=	2	Z2	=	5			
S1 - S1	COULOMB (M-M)	**	Z1	=	3	Z2	=	3			
S1 - S2	COULOMB (M-M)	**	Z1	=	3	Z2	=	3			
S1 - 01	SPRINGS	1	LONG	=	15	TRANS	=	16			
	COULOMB (M-M)	**	Z1	=	3	Z2	=	4			
S1 - 05	COULOMB (M-M)	**	Z1	=	3	Z2	=	4			
S1 - 02	SPRINGS	1	LONG	=	17	TRANS	=	18			
	COULOMB (M-M)	**	Z1	=	3	Z2	=	5			
S1 - 06	COULOMB (M-M)	**	Z1	=	3	Z2	=	5			
S1 - 03	SPRINGS	1	LONG	=	17	TRANS	=	18			
	COULOMB (M-M)	**	Z1	=	3	Z2	=	5			
S1 - 07	COULOMB (M-M)	**	Z1	=	3	Z2	=	5			
S1 - 04	SPRINGS	1	LONG	=	17	TRANS	=	18			
	COULOMB (M-M)	**	Z1	=	3	Z2	=	5			
S1 - 08	COULOMB (M-M)	**	Z1	=	3	Z2	=	5			
S2 - S2	COULOMB (M-M)	**	Z1	=	3	Z2	=	3			
S2 - 01	COULOMB (M-M)	**	Z1	=	3	Z2	=	4			
S2 - 05	SPRINGS	1	LONG	=	15	TRANS	=	16			
	COULOMB (M-M)	**	Z1	=	3	Z2	=	4			
S2 - 02	COULOMB (M-M)	**	Z1	=	3	Z2	=	5			
S2 - 06	SPRINGS	1	LONG	=	17	TRANS	=	18			
	COULOMB (M-M)	**	Z1	=	3	Z2	=	5			
S2 - 03	COULOMB (M-M)	**	Z1	=	3	Z2	=	5			
S2 - 07	SPRINGS	1	LONG	=	17	TRANS	=	18			
	COULOMB (M-M)	**	Z1	=	3	Z2	=	5			
S2 - 04	COULOMB (M-M)	**	Z1	=	3	Z2	=	5			
S2 - 08	SPRINGS	1	LONG	=	17	TRANS	=	18			
	COULOMB (M-M)	**	Z1	=	3	Z2	=	5			
01 - 01	COULOMB (M-M)	**	Z1	=	4	Z2	=	4			
01 - 05	COULOMB (M-M)	**	Z1	=	4	Z2	=	4			
01 - 02	SPRINGS	1	LONG	=	11	TRANS	=	12			
	COULOMB (M-M)	**	Z1	=	4	Z2	=	5			
01 - 06	COULOMB (M-M)	**	Z1	=	4	Z2	=	5			
01 - 03	SPRINGS	1	LONG	=	11	TRANS	=	12			
	COULOMB (M-M)	**	Z1	=	4	Z2	=	5			
01 - 07	COULOMB (M-M)	**	Z1	=	4	Z2	=	5			
01 - 04	SPRINGS	1	LONG	=	11	TRANS	=	12			
	COULOMB (M-M)	**	Z1	=	4	Z2	=	5			
01 - 08	COULOMB (M-M)	**	Z1	=	4	Z2	=	5			
05 - 05	COULOMB (M-M)	**	Z1	=	4	Z2	=	4			
05 - 02	COULOMB (M-M)	**	Z1	=	4	Z2	=	5			
05 - 06	SPRINGS	1	LONG	=	11	TRANS	=	12			
	COULOMB (M-M)	**	Z1	=	4	Z2	=	5			
05 - 03	COULOMB (M-M)	**	Z1	=	4	Z2	=	5			
05 - 07	SPRINGS	1	LONG	=	11	TRANS	=	12			
	COULOMB (M-M)	**	Z1	=	4	Z2	=	5			
05 - 04	COULOMB (M-M)	**	Z1	=	4	Z2	=	5			
05 - 08	SPRINGS	1	LONG	=	11	TRANS	=	12			
	COULOMB (M-M)	**	Z1	=	4	Z2	=	5			

02	- 02	COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
02	- 06	COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
02	- 03	SPRINGS	1	LONG	=	13	TRANS	=	14	
		COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
02	- 07	COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
02	- 04	SPRINGS	1	LONG	=	13	TRANS	=	14	
		COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
02	- 08	COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
06	- 06	COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
06	- 03	COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
06	- 07	SPRINGS	1	LONG	=	13	TRANS	=	14	
		COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
06	- 04	COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
06	- 08	SPRINGS	1	LONG	=	13	TRANS	=	14	
		COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
03	- 03	COULOMB (M-M)	**	Z1	=	5	Z	=	5	
03	- 07	COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
03	- 04	SPRINGS	1	LONG	=	13	TRANS	=	14	
		COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
03	- 08	COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
07	- 07	COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
07	- 04	COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
07	- 08	SPRINGS	1	LONG	=	13	TRANS	=	14	
		COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
04	- 04	COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
04	- 08	COULOMB (M-M)	**	Z1	=	5	Z2	=	5	
08	- 08	COULOMB (M-M)	**	Z1	=	5	Z2	=	5	

PARAMETER-VALUES :

PAR.-NO.	VALUE	
1	1.200	E
2	0.400	E
3	1.350	E
4	-0.850	E
5	-0.700	E
6	0.197	A
7	0.086	A
8	0.106	A
9	0.100	A
10	2000.000	EV
11	250.000	N/M
12	-0.500	N/M
13	250.000	N/M
14	-0.300	N/M
15	700.000	N/M
16	-53.800	N/M
17	700.000	N/M
18	-38.600	N/M

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********** Q = ( 0.0 , 0.0 , 0.00) 1/A ********** QHKL = ( 0.0 , 0.0 , 0.00) **********

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EIGENVALUES AND EIGENVECTORS FOR IRM  1

NY**2 =   -0.0022 THZ**2    NEGATIV !!!

   K1              0.0       0.0          0.0       0.0          0.370899 0.000001
   K2              0.0       0.0          0.0       0.0          0.370899 0.000001
   L11             0.0       0.0          0.0       0.0          0.156264 0.000000
   L12             0.0       0.0          0.0       0.0          0.156264 0.000000
   S1              0.0       0.0          0.0       0.0          0.335878 0.000001
   S2              0.0       0.0          0.0       0.0          0.335878 0.000001
   01              0.0       0.0          0.0       0.0          0.237277 0.000001
   05              0.0       0.0          0.0       0.0          0.237277 0.000001
   02              0.000000  0.000000    -0.000001-0.000000     0.237278 0.000001
   06             -0.000000-0.000000     0.000001  0.000000     0.237278 0.000001
   03              0.000000  0.000000     0.000001  0.000000     0.237278 0.000001
   07             -0.000000-0.000000    -0.000001-0.000000     0.237278 0.000001
   04             -0.000001-0.000000     0.000000-0.000000     0.237278 0.000001
   08              0.000001  0.000000    -0.000000  0.000000     0.237278 0.000001
NY =  4.59 THZ

   K1              0.0       0.0          0.0       0.0          0.166906 0.000000
   K2              0.0       0.0          0.0       0.0          0.166906 0.000000
   L11             0.0       0.0          0.0       0.0         -0.098170-0.000000
   L12             0.0       0.0          0.0       0.0         -0.098170-0.000000
   S1              0.0       0.0          0.0       0.0         -0.054130-0.000000
   S2              0.0       0.0          0.0       0.0         -0.054130-0.000000
   01              0.0       0.0          0.0       0.0         -0.035684-0.000000
   05              0.0       0.0          0.0       0.0         -0.035684-0.000000
   02             -0.011828-0.000000    -0.389674-0.000001     -0.027981-0.000000
   06              0.011828  0.000000     0.389674  0.000001     -0.027981-0.000000
   03              0.343381  0.000001     0.184593-0.000000     -0.027981-0.000000
   07             -0.343381-0.000001    -0.184593-0.000001     -0.027981-0.000000
   04             -0.331553-0.000001     0.205079  0.000000     -0.027981-0.000000
   08              0.331553  0.000001    -0.205079-0.000000     -0.027981-0.000000
NY =  6.17 THZ

   K1              0.0       0.0          0.0       0.0          0.556919 0.000002
   K2              0.0       0.0          0.0       0.0          0.556919 0.000002
   L11             0.0       0.0          0.0       0.0         -0.243653-0.000001
   L12             0.0       0.0          0.0       0.0         -0.243653-0.000001
   S1              0.0       0.0          0.0       0.0         -0.208330-0.000001
   S2              0.0       0.0          0.0       0.0         -0.208330-0.000001
   01              0.0       0.0          0.0       0.0         -0.120520-0.000000
   05              0.0       0.0          0.0       0.0         -0.120520-0.000000
   02              0.011675  0.000000     0.119999  0.000000    -0.098219-0.000000
   06             -0.011675-0.000000    -0.119999-0.000000     -0.098219-0.000000
   03             -0.109759-0.000000    -0.049888  0.000000     -0.098219-0.000000
   07              0.109759  0.000000     0.049888  0.000000     -0.098219-0.000000
   04              0.098084  0.000000    -0.070110-0.000000     -0.098219-0.000000
   08             -0.098084-0.000000     0.070110  0.000000     -0.098219-0.000000
NY =  9.79 THZ

   K1              0.0       0.0          0.0       0.0         -0.140773-0.000000
   K2              0.0       0.0          0.0       0.0         -0.140773-0.000000
   L11             0.0       0.0          0.0       0.0         -0.633386-0.000002
   L12             0.0       0.0          0.0       0.0         -0.633386-0.000002
   S1              0.0       0.0          0.0       0.0          0.229659 0.000001
   S2              0.0       0.0          0.0       0.0          0.229659 0.000001
   01              0.0       0.0          0.0       0.0          0.101603 0.000000
   05              0.0       0.0          0.0       0.0          0.101603 0.000000
   02             -0.013201-0.000000     0.014717  0.000000     0.070160 0.000000
   06              0.013201  0.000000    -0.014717-0.000000     0.070160 0.000000
   03             -0.006145-0.000000    -0.018791-0.000000     0.070160 0.000000
   07              0.006145  0.000000     0.018791  0.000000     0.070160 0.000000
   04              0.019346  0.000000     0.004074  0.000000     0.070160 0.000000
   08             -0.019346-0.000000    -0.004074-0.000000     0.070160 0.000000
NY =  18.04 THZ

   K1              0.0       0.0          0.0       0.0          0.066148 0.000000
   K2              0.0       0.0          0.0       0.0          0.066148 0.000000
   L11             0.0       0.0          0.0       0.0          0.069804 0.000000
   L12             0.0       0.0          0.0       0.0          0.069804 0.000000
   S1              0.0       0.0          0.0       0.0          0.419982 0.000001
   S2              0.0       0.0          0.0       0.0          0.419982 0.000001
   01              0.0       0.0          0.0       0.0          0.109886 0.000000
   05              0.0       0.0          0.0       0.0          0.109886 0.000000
   02             -0.140514-0.000000     0.005481  0.000000    -0.284586-0.000001
   06              0.140514  0.000000    -0.005481-0.000000     -0.284586-0.000001
   03              0.065510-0.000000    -0.124429-0.000000     -0.284586-0.000001
   07             -0.065510-0.000000     0.124429  0.000000    -0.284586-0.000001
   04              0.075004  0.000000     0.118948  0.000000    -0.284586-0.000001
   08             -0.075004-0.000000    -0.118948-0.000000     -0.284586-0.000001
NY =  33.79 THZ

   K1              0.0       0.0          0.0       0.0          0.015037 0.000000
   K2              0.0       0.0          0.0       0.0          0.015037 0.000000
   L11             0.0       0.0          0.0       0.0          0.022797 0.000000
   L12             0.0       0.0          0.0       0.0          0.022797 0.000000
   S1              0.0       0.0          0.0       0.0          0.334099 0.000001
   S2              0.0       0.0          0.0       0.0          0.334099 0.000001
   01              0.0       0.0          0.0       0.0         -0.537872-0.000002
   05              0.0       0.0          0.0       0.0         -0.537872-0.000002
   02              0.180758  0.000000    -0.004938-0.000000     0.008807 0.000000
   06             -0.180758-0.000000     0.004938  0.000000     0.008807 0.000000
   03             -0.086102  0.000000     0.159010  0.000000     0.008807 0.000000
   07              0.086102  0.000000    -0.159010-0.000000     0.008807 0.000000
   04             -0.094655-0.000000    -0.154072-0.000000     0.008807 0.000000
   08              0.094655  0.000000     0.154072  0.000000     0.008807 0.000000
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NY = 39.57 THZ

   K1          0.0      0.0          0.0      0.0          0.000564 0.000000
   K2          0.0      0.0          0.0      0.0          0.000564 0.000000
   LI1         0.0      0.0          0.0      0.0         -0.002936-0.000000
   LI2         0.0      0.0          0.0      0.0         -0.002936-0.000000
   S1          0.0      0.0          0.0      0.0          0.010216 0.000000
   S2          0.0      0.0          0.0      0.0          0.010216 0.000000
   01          0.0      0.0          0.0      0.0          0.340877 0.000001
   05          0.0      0.0          0.0      0.0          0.340877 0.000001
   02          0.337341 0.000001    -0.012311-0.000000    -0.118095-0.000000
   06         -0.337341-0.000001     0.012311 0.000000    -0.118095-0.000000
   03         -0.158009 0.000000     0.298301 0.000001    -0.118095-0.000000
   07          0.158009 0.000001    -0.298301-0.000001    -0.118095-0.000000
   04         -0.179332-0.000000    -0.285990-0.000001    -0.118095-0.000000


   08          0.179332 0.000000     0.285990 0.000001    -0.118095-0.000000
EIGENVALUES AND EIGENVECTORS FOR IRM  2

(2-FOLD DEGENERATE)
NY**2 =   -0.0016 THZ**2    NEGATIV !!!

   K1         -0.262244-0.000002     0.000001-0.262244     0.0      0.0
   K2         -0.262244-0.000001     0.000001-0.262243     0.0      0.0
   LI1        -0.110499 0.000003    -0.000004-0.110499     0.0      0.0
   LI2        -0.110500 0.000004    -0.000004-0.110499     0.0      0.0
   S1         -0.237505 0.000003    -0.000004-0.237505     0.0      0.0
   S2         -0.237506 0.000004    -0.000004-0.237505     0.0      0.0
   01         -0.167750 0.000007    -0.000008-0.167750     0.0      0.0
   05         -0.167750 0.000008    -0.000008-0.167749     0.0      0.0
   02         -0.167799 0.000000    -0.000001-0.167798    -0.000037-0.000004
   06         -0.167800 0.000001    -0.000002-0.167799     0.000037 0.000004
   03         -0.167799 0.000003    -0.000001-0.167798     0.000023-0.000030
   07         -0.167799 0.000002    -0.000000-0.167798    -0.000023 0.000030
   04         -0.167798 0.000001    -0.000001-0.167799     0.000015 0.000035
   08         -0.167798 0.000001    -0.000002-0.167800    -0.000015-0.000035
NY =  2.07 THZ

   K1          0.100978 0.000001    -0.000000 0.100978     0.0      0.0
   K2          0.100978 0.000000    -0.000000 0.100978     0.0      0.0
   LI1        -0.018594 0.008533    -0.008534-0.018594     0.0      0.0
   LI2        -0.018594 0.008534    -0.008534-0.018594     0.0      0.0
   S1         -0.029070-0.002151     0.002151-0.029070     0.0      0.0
   S2         -0.029070-0.002151     0.002151-0.029070     0.0      0.0
   01          0.192528 0.191899    -0.191899 0.192529     0.0      0.0
   05          0.192529 0.191899    -0.191898 0.192529     0.0      0.0
   02         -0.097736-0.066729     0.062853-0.100134    -0.222742-0.179348
   06         -0.097736-0.066728     0.062853-0.100135     0.222743 0.179347
   03         -0.101213-0.064860     0.064721-0.096658     0.266690-0.103227
   07         -0.101213-0.064860     0.064721-0.096657    -0.266690 0.103226
   04         -0.097857-0.062783     0.066798-0.100013    -0.043948 0.282574
   08         -0.097857-0.062783     0.066798-0.100014     0.043947-0.282575
NY =  4.23 THZ

   K1         -0.412623-0.000002     0.000002-0.412623     0.0      0.0
   K2         -0.412624-0.000002     0.000001-0.412623     0.0      0.0
   LI1         0.034138 0.002072    -0.002072 0.034138     0.0      0.0
   LI2         0.034138 0.002072    -0.002072 0.034138     0.0      0.0
   S1          0.142177-0.000886     0.000887 0.142177     0.0      0.0
   S2          0.142178-0.000887     0.000887 0.142177     0.0      0.0
   01          0.159985 0.048715    -0.048714 0.159985     0.0      0.0
   05          0.159986 0.048715    -0.048714 0.159985     0.0      0.0
   02          0.085203-0.015677     0.016863 0.088948    -0.053199-0.041563
   06          0.085203-0.015677     0.016864 0.088948     0.053200 0.041563
   03          0.088525-0.014945     0.017596 0.085625     0.062594-0.025291
   07          0.088525-0.014945     0.017596 0.085625    -0.062594 0.025290
   04          0.087498-0.018189     0.014352 0.086653    -0.009395 0.066854
   08          0.087498-0.018189     0.014352 0.086653     0.009395-0.066854
NY =  8.60 THZ

   K1          0.026723 0.000000    -0.000000 0.026723     0.0      0.0
   K2          0.026723 0.000000    -0.000000 0.026723     0.0      0.0
   LI1        -0.485898-0.002407     0.002406-0.485898     0.0      0.0
   LI2        -0.485899-0.002406     0.002405-0.485897     0.0      0.0
   S1          0.068345 0.003782    -0.003781 0.068345     0.0      0.0
   S2          0.068345 0.003781    -0.003781 0.068345     0.0      0.0
   01          0.047134-0.009331     0.009331 0.047134     0.0      0.0
   05          0.047134-0.009331     0.009331 0.047134     0.0      0.0
   02          0.047032 0.005266     0.001557 0.042535     0.003771 0.007725
   06          0.047032 0.005266     0.001557 0.042535    -0.003771-0.007725
   03          0.046614-0.001799    -0.005508 0.042953    -0.008575-0.000597
   07          0.046614-0.001799    -0.005508 0.042953     0.008575 0.000597
   04          0.040705 0.002096    -0.001613 0.048863     0.004804-0.007128
   08          0.040705 0.002096    -0.001613 0.048863    -0.004804 0.007128
NY = 16.51 THZ

   K1         -0.002880-0.000000     0.000000-0.002880     0.0      0.0
   K2         -0.002880-0.000000     0.000000-0.002880     0.0      0.0
   LI1         0.001239-0.007047     0.007047 0.001239     0.0      0.0
   LI2         0.001239-0.007047     0.007047 0.001239     0.0      0.0
   S1          0.034513-0.070226     0.070226 0.034513     0.0      0.0
   S2          0.034513-0.070226     0.070226 0.034513     0.0      0.0
   01          0.165786-0.113275     0.113275 0.165785     0.0      0.0
   05          0.165786-0.113275     0.113275 0.165785     0.0      0.0
   02          0.055931-0.071284    -0.216168-0.196568     0.157163-0.131868
   06          0.055931-0.071284    -0.216170-0.196567    -0.157162 0.131869
   03         -0.257913 0.034972    -0.109914 0.117278     0.035621 0.202041
   07         -0.257913 0.034971    -0.109914 0.117277    -0.035620-0.202041
   04         -0.008972 0.253640     0.108756-0.131664    -0.192783-0.070172
   08         -0.008971 0.253640     0.108755-0.131665     0.192783 0.070172
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NY = 17.15 THZ

   K1              0.007159 0.000000   -0.000000 0.007159    0.0       0.0
   K2              0.007159 0.000000   -0.000000 0.007159    0.0       0.0
   L11            -0.003373 0.005415   -0.005415-0.003373    0.0       0.0
   L12            -0.003373 0.005415   -0.005415-0.003373    0.0       0.0
   S1             -0.319344-0.073236    0.073236-0.319344    0.0       0.0
   S2             -0.319345-0.073236    0.073235-0.319344    0.0       0.0
   01              0.256113 0.087926   -0.087926 0.256113    0.0       0.0
   05              0.256113 0.087926   -0.087925 0.256112    0.0       0.0
   02             -0.033933 0.004424   -0.003693 0.158570    0.133145 0.045852
   06             -0.033933 0.004424   -0.003693 0.158570   -0.133145-0.045852
   03              0.110761 0.087232    0.079115 0.013876   -0.106281 0.092381
   07              0.110761 0.087232    0.079115 0.013876    0.106282-0.092381
   04              0.110128-0.079481   -0.087598 0.014509   -0.026864-0.138233
   08              0.110127-0.079481   -0.087598 0.014510    0.026864 0.138233
NY = 34.21 THZ

   K1              0.000617 0.000000   -0.000000 0.000617    0.0       0.0
   K2              0.000617 0.000000   -0.000000 0.000617    0.0       0.0
   L11            -0.002333-0.000726    0.000726-0.002333    0.0       0.0
   L12            -0.002333-0.000726    0.000726-0.002333    0.0       0.0
   S1             -0.200576 0.118925   -0.118926-0.200576    0.0       0.0
   S2             -0.200576 0.118926   -0.118926-0.200575    0.0       0.0
   01             -0.055802 0.030581   -0.030581-0.055802    0.0       0.0
   05             -0.055802 0.030581   -0.030581-0.055802    0.0       0.0
   02              0.273212-0.175312   -0.043017-0.046349   -0.114490 0.072304
   06              0.273212-0.175314   -0.043017-0.046349    0.114490-0.072305
   03             -0.060999-0.149939   -0.017642 0.287861   -0.005373-0.135303
   07             -0.060998-0.149939   -0.017643 0.287861    0.005373 0.135303
   04              0.128081 0.126808    0.259104 0.098782    0.119863 0.062998
NY**2 =    -0.0016 THZ**2    NEGATIV !!!
   08              0.128081 0.126808    0.259105 0.098781   -0.119863-0.062998
   K1             -0.262243 0.0         0.0      0.262243    0.0       0.0
   K2             -0.262243 0.0         0.0      0.262243    0.0       0.0
   L11            -0.110498-0.000008   -0.000008 0.110498    0.0       0.0
   L12            -0.110498-0.000008   -0.000008 0.110498    0.0       0.0
   S1             -0.237506-0.000014   -0.000014 0.237506    0.0       0.0
   S2             -0.237506-0.000014   -0.000014 0.237506    0.0       0.0
   01             -0.167734-0.000004   -0.000004 0.167734    0.0       0.0
   05             -0.167734-0.000004   -0.000004 0.167734    0.0       0.0
   02             -0.167805-0.000012   -0.000013 0.167803   -0.000052-0.000009
   06             -0.167806-0.000012   -0.000013 0.167804    0.000052 0.000009
   03             -0.167804-0.000014   -0.000012 0.167804    0.000019 0.000050
   07             -0.167804-0.000014   -0.000012 0.167804   -0.000019-0.000050
   04             -0.167803-0.000012   -0.000013 0.167805    0.000034-0.000041
   08             -0.167803-0.000012   -0.000013 0.167805   -0.000034 0.000041
NY =  2.07 THZ

   K1              0.100977 0.0         0.0     -0.100977    0.0       0.0
   K2              0.100977 0.0         0.0     -0.100977    0.0       0.0
   L11            -0.018589-0.008543   -0.008543 0.018589    0.0       0.0
   L12            -0.018589-0.008543   -0.008543 0.018589    0.0       0.0
   S1             -0.029066 0.002129    0.002129 0.029066    0.0       0.0
   S2             -0.029066 0.002129    0.002129 0.029066    0.0       0.0
   01              0.192554-0.191891   -0.191891-0.192554    0.0       0.0
   05              0.192554-0.191891   -0.191891-0.192554    0.0       0.0
   02             -0.097740 0.066705    0.062829 0.100139   -0.222762 0.179324
   06             -0.097740 0.066705    0.062829 0.100139    0.222762-0.179324
   03             -0.101218 0.064837    0.064697 0.096662    0.266680 0.103256
   07             -0.101218 0.064837    0.064697 0.096662   -0.266680-0.103256
   04             -0.097861 0.062759    0.066775 0.100018   -0.043918-0.282579
   08             -0.097861 0.062759    0.066775 0.100018    0.043919 0.282580
NY =  4.23 THZ

   K1             -0.412624 0.0         0.0      0.412624    0.0       0.0
   K2             -0.412624 0.0         0.0      0.412624    0.0       0.0
   L11             0.034139-0.002072   -0.002072-0.034139    0.0       0.0
   L12             0.034139-0.002072   -0.002072-0.034139    0.0       0.0
   S1              0.142179 0.000888    0.000888-0.142179    0.0       0.0
   S2              0.142179 0.000888    0.000888-0.142179    0.0       0.0
   01              0.159981-0.048715   -0.048715-0.159981    0.0       0.0
   05              0.159981-0.048715   -0.048715-0.159981    0.0       0.0
   02              0.085205 0.015679    0.016865-0.088950   -0.053195 0.041565
   06              0.085205 0.015679    0.016865-0.088950    0.053195-0.041565
   03              0.088527 0.014947    0.017597-0.085627    0.062594 0.025285
   07              0.088527 0.014947    0.017597-0.085627   -0.062594-0.025285
   04              0.087500 0.018190    0.014354-0.086655   -0.009399-0.066850
   08              0.087500 0.018190    0.014354-0.086655    0.009399 0.066851
NY =  8.60 THZ

   K1              0.026723 0.0         0.0     -0.026723    0.0       0.0
   K2              0.026723 0.0         0.0     -0.026723    0.0       0.0
   L11            -0.485899 0.002407    0.002407 0.485899    0.0       0.0
   L12            -0.485899 0.002407    0.002407 0.485899    0.0       0.0
   S1              0.068344-0.003781   -0.003781-0.068344    0.0       0.0
   S2              0.068344-0.003781   -0.003781-0.068344    0.0       0.0
   01              0.047136 0.009330    0.009330-0.047136    0.0       0.0
   05              0.047136 0.009330    0.009330-0.047136    0.0       0.0
   02              0.047032-0.005265    0.001557-0.042535    0.003769-0.007723
   06              0.047032-0.005265    0.001557-0.042535   -0.003769 0.007723
   03              0.046614 0.001799   -0.005507-0.042953   -0.008573 0.000598
   07              0.046614 0.001799   -0.005507-0.042953    0.008573-0.000598
   04              0.040705-0.002096   -0.001612-0.048862    0.004804 0.007126
   08              0.040705-0.002096   -0.001612-0.048862   -0.004804-0.007126
NY = 16.51 THZ

   K1             -0.002880 0.0         0.0      0.002880    0.0       0.0
   K2             -0.002880 0.0         0.0      0.002880    0.0       0.0
   L11             0.001237 0.007047    0.007047-0.001237    0.0       0.0
   L12             0.001237 0.007047    0.007047-0.001237    0.0       0.0
   S1              0.034495 0.070237    0.070237-0.034495    0.0       0.0
   S2              0.034495 0.070237    0.070237-0.034495    0.0       0.0
   01              0.165780 0.113287    0.113287-0.165780    0.0       0.0
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    O5              0.165780 0.113287    0.113287-0.165780    0.0      0.0
    O2              0.055922 0.071291   -0.216193 0.196539    0.157153 0.131882
    O6              0.055923 0.071291   -0.216194 0.196540   -0.157153-0.131882
    O3             -0.257908-0.035003   -0.109899-0.117292    0.035637-0.202039
    O7             -0.257908-0.035003   -0.109899-0.117291   -0.035637 0.202039
    O4             -0.008939-0.253641    0.108739 0.131678   -0.192789 0.070157
    O8             -0.008939-0.253641    0.108739 0.131678    0.192789-0.070158
NY = 17.15 THZ

    K1              0.007159 0.0         0.0     -0.007159    0.0      0.0
    K2              0.007159 0.0         0.0     -0.007159    0.0      0.0
    L11            -0.003372-0.005415   -0.005415 0.003372    0.0      0.0
    L12            -0.003372-0.005415   -0.005415 0.003372    0.0      0.0
    S1             -0.319343 0.073239    0.073239 0.319343    0.0      0.0
    S2             -0.319343 0.073239    0.073239 0.319343    0.0      0.0
    O1              0.256109-0.087937   -0.087937-0.256109    0.0      0.0
    O5              0.256109-0.087937   -0.087937-0.256109    0.0      0.0
    O2             -0.033933-0.004427   -0.003685-0.158574    0.133140-0.045862
    O6             -0.033934-0.004427   -0.003685-0.158574   -0.133140 0.045862
    O3              0.110768-0.087229    0.079117-0.013872   -0.106288-0.092372
    O7              0.110768-0.087228    0.079117-0.013872    0.106288 0.092372
    O4              0.110126 0.079488   -0.087600-0.014515   -0.026853 0.138234
    O8              0.110126 0.079488   -0.087600-0.014515    0.026853-0.138234
NY = 34.21 THZ

    K1              0.000617 0.0         0.0     -0.000617    0.0      0.0
    K2              0.000617 0.0         0.0     -0.000617    0.0      0.0
    L11            -0.002332 0.000727    0.000727 0.002332    0.0      0.0
    L12            -0.002332 0.000727    0.000727 0.002332    0.0      0.0
    S1             -0.200599-0.118888   -0.118888 0.200599    0.0      0.0
    S2             -0.200599-0.118888   -0.118888 0.200599    0.0      0.0
    O1             -0.055809-0.030571   -0.030571 0.055809    0.0      0.0
    O5             -0.055809-0.030571   -0.030571 0.055809    0.0      0.0
    O2              0.273245 0.175261   -0.043008 0.046357   -0.114504-0.072283
    O6              0.273245 0.175262   -0.043008 0.046357    0.114504 0.072283
    O3             -0.060970 0.149951   -0.017698-0.287858   -0.005348 0.135305
    O7             -0.060970 0.149951   -0.017697-0.287858    0.005348-0.135305
    O4              0.128057-0.126832    0.259086-0.098831    0.119851-0.063021
    O8              0.128057-0.126832    0.259086-0.098831   -0.119851 0.063021
EIGENVALUES AND EIGENVECTORS FOR IRM  3

(2-FOLD DEGENERATE)
NY =  1.62 THZ

    K1             -0.164003-0.000001   -0.000000 0.164003    0.0      0.0
    K2              0.164003 0.000000    0.000000-0.164003    0.0      0.0
    L11            -0.034164 0.083533    0.083533 0.034164    0.0      0.0
    L12             0.034164-0.083533   -0.083533-0.034164    0.0      0.0
    S1              0.062814-0.174448   -0.174448-0.062814    0.0      0.0
    S2             -0.062814 0.174448    0.174448 0.062814    0.0      0.0
    O1             -0.025082 0.054381    0.054381 0.025082    0.0      0.0
    O5              0.025082-0.054381   -0.054381-0.025082    0.0      0.0
    O2              0.067473-0.188347   -0.189385-0.068384    0.072999-0.179155
    O6             -0.067472 0.188347    0.189386 0.068384    0.072999-0.179155
    O3              0.067706-0.189521   -0.188212-0.068150   -0.191652 0.026359
    O7             -0.067706 0.189520    0.188212 0.068150   -0.191652 0.026359
    O4              0.068606-0.188732   -0.189001-0.067251    0.118654 0.152796
    O8             -0.068605 0.188731    0.189001 0.067250    0.118654 0.152796
NY =  2.93 THZ

    K1             -0.327989-0.000001   -0.000001 0.327989    0.0      0.0
    K2              0.327988 0.000001    0.000001-0.327989    0.0      0.0
    L11             0.012289-0.030992   -0.030992-0.012289    0.0      0.0
    L12            -0.012289 0.030992    0.030992 0.012289    0.0      0.0
    S1              0.048249 0.178536    0.178536-0.048249    0.0      0.0
    S2             -0.048249-0.178536   -0.178536 0.048249    0.0      0.0
    O1              0.108108 0.220873    0.220873-0.108108    0.0      0.0
    O5             -0.108108-0.220873   -0.220874 0.108109    0.0      0.0
    O2              0.007507 0.091820    0.091091 0.000069   -0.067659-0.098634
    O6             -0.007507-0.091820   -0.091091-0.000069   -0.067659-0.098633
    O3              0.001509 0.094554    0.088357-0.005928   -0.051590 0.107911
    O7             -0.001509-0.094554   -0.088357 0.005928   -0.051590 0.107911
    O4              0.002140 0.087993    0.094918-0.005297    0.119249-0.009278
    O8             -0.002141-0.087993   -0.094918 0.005298    0.119248-0.009278
NY =  3.88 THZ

    K1              0.338528 0.000001    0.000001-0.338528    0.0      0.0
    K2             -0.338528-0.000001   -0.000001 0.338529    0.0      0.0
    L11            -0.044611 0.017532    0.017532 0.044611    0.0      0.0
    L12             0.044611-0.017532   -0.017533-0.044612    0.0      0.0
    S1              0.072707 0.086613    0.086612-0.072707    0.0      0.0
    S2             -0.072707-0.086612   -0.086613 0.072707    0.0      0.0
    O1              0.084464 0.245280    0.245279-0.084464    0.0      0.0
    O5             -0.084464-0.245279   -0.245280 0.084464    0.0      0.0
    O2              0.035516-0.002055   -0.003492-0.035933   -0.040404-0.176474
    O6             -0.035516 0.002055    0.003492 0.035933   -0.040405-0.176473
    O3              0.035206-0.003313   -0.002234-0.036243   -0.132628 0.123229
    O7             -0.035206 0.003313    0.002234 0.036243   -0.132628 0.123228
    O4              0.036451-0.002952   -0.002595-0.034998    0.173033 0.053245
    O8             -0.036451 0.002953    0.002595 0.034998    0.173033 0.053245
NY =  8.54 THZ

    K1              0.028613 0.000000    0.000000-0.028613    0.0      0.0
    K2             -0.028613-0.000000   -0.000000 0.028613    0.0      0.0
    L11             0.479264-0.088700   -0.088701-0.479264    0.0      0.0
    L12            -0.479264 0.088701    0.088701 0.479265    0.0      0.0
    S1              0.036492-0.008704   -0.008704-0.036492    0.0      0.0
    S2             -0.036492 0.008704    0.008704 0.036492    0.0      0.0
    O1              0.021423 0.010564    0.010564-0.021423    0.0      0.0
    O5             -0.021423-0.010564   -0.010564 0.021423    0.0      0.0
    O2              0.044963-0.014087   -0.006049-0.041157    0.045969-0.019064
    O6             -0.044963 0.014087    0.006050 0.041157    0.045969-0.019064
    O3              0.045589-0.006411   -0.013726-0.040531   -0.039494-0.030278
    O7             -0.045589 0.006411    0.013726 0.040531   -0.039494-0.030278
    O4              0.038628-0.009707   -0.010430-0.047492   -0.006475 0.049342
    O8             -0.038628 0.009707    0.010430 0.047492   -0.006475 0.049342
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NY =  16.37 THZ

   K1          0.009137 0.000000   0.000000-0.009137   0.0       0.0
   K2         -0.009137-0.000000  -0.000000 0.009137   0.0       0.0
   LI1        -0.021816 0.005221   0.005221 0.021816   0.0       0.0
   LI2         0.021816-0.005221  -0.005221-0.021816   0.0       0.0
   S1          0.021773-0.033302  -0.033302-0.021773   0.0       0.0
   S2         -0.021773 0.033302   0.033302 0.021773   0.0       0.0
   01          0.208691-0.085923  -0.085924-0.208691   0.0       0.0
   05         -0.208691 0.085924   0.085924 0.208691   0.0       0.0
   02          0.078911-0.030391   0.117018 0.248631   0.203217-0.085468
   06         -0.078912 0.030391  -0.117019-0.248631   0.203217-0.085469
   03         -0.102915 0.221997  -0.135368 0.066805  -0.175627-0.133256
   07          0.102915-0.221997   0.135369-0.066804  -0.175627-0.133257
   04         -0.230576-0.061664   0.148291-0.060856  -0.027590 0.218725
   08          0.230576 0.061663  -0.148291 0.060857  -0.027590 0.218725
NY =  17.21 THZ

   K1          0.004454 0.000000   0.000000-0.004454   0.0       0.0
   K2         -0.004454-0.000000  -0.000000 0.004454   0.0       0.0
   LI1         0.003655 0.018961   0.018961-0.003655   0.0       0.0
   LI2        -0.003655-0.018961  -0.018961 0.003655   0.0       0.0
   S1         -0.013711 0.332985   0.332985 0.013710   0.0       0.0
   S2          0.013710-0.332985  -0.332986-0.013710   0.0       0.0
   01          0.031577-0.249593  -0.249593-0.031576   0.0       0.0
   05         -0.031576 0.249593   0.249594 0.031576   0.0       0.0
   02         -0.005856 0.044976  -0.187782-0.003770   0.020044-0.111484
   06          0.005856-0.044976   0.187782 0.003769   0.020044-0.111484
   03         -0.099424-0.133760  -0.009046-0.097338  -0.106570 0.038384
   07          0.099424 0.133761   0.009045 0.097338  -0.106570 0.038384
   04          0.102150-0.125425  -0.017381 0.104237   0.086526 0.073100
   08         -0.102150 0.125425   0.017381-0.104237   0.086526 0.073100
NY =  34.20 THZ

   K1          0.001921 0.000000   0.000000-0.001921   0.0       0.0
   K2         -0.001921-0.000000  -0.000000 0.001921   0.0       0.0
   LI1        -0.000351 0.002747   0.002747 0.000351   0.0       0.0
   LI2         0.000351-0.002747  -0.002747-0.000351   0.0       0.0
   S1          0.172469-0.157569  -0.157569-0.172469   0.0       0.0
   S2         -0.172469 0.157569   0.157569 0.172469   0.0       0.0
   01          0.047270-0.040129  -0.040129-0.047270   0.0       0.0
   05         -0.047270 0.040129   0.040129 0.047270   0.0       0.0
   02         -0.248174 0.209448  -0.031557-0.054854   0.102752-0.087703
   06          0.248174-0.209450   0.031557 0.054854   0.102752-0.087703
   03         -0.125262-0.102520   0.280412 0.068058  -0.127330-0.045134
   07          0.125261 0.102520  -0.280412-0.068058  -0.127329-0.045134
   04          0.083455 0.159909   0.017983 0.276776   0.024577 0.132838
   08         -0.083457-0.159909  -0.017983-0.276775   0.024578 0.132837
NY =   1.62 THZ

   K1         -0.164013-0.000000   0.000000-0.164013   0.0       0.0
   K2          0.164013 0.000000  -0.000000 0.164013   0.0       0.0
   LI1        -0.034149-0.083537   0.083537-0.034149   0.0       0.0
   LI2         0.034149 0.083537  -0.083537 0.034149   0.0       0.0
   S1          0.062773 0.174446  -0.174446 0.062773   0.0       0.0
   S2         -0.062773-0.174446   0.174446-0.062773   0.0       0.0
   01         -0.025087-0.054407   0.054407-0.025087   0.0       0.0
   05          0.025087 0.054407  -0.054407 0.025087   0.0       0.0
   02          0.067433 0.188354  -0.189393 0.068345   0.072973 0.179179
   06         -0.067433-0.188354   0.189393-0.068345   0.072973 0.179179
   03          0.067667 0.189527  -0.188219 0.068112  -0.191661-0.026393
   07         -0.067667-0.189528   0.188219-0.068111  -0.191661-0.026393
   04          0.068567 0.188739  -0.189009 0.067212   0.118688-0.152786
   08         -0.068567-0.188738   0.189008-0.067212   0.118688-0.152786
NY =   2.93 THZ

   K1         -0.327961-0.000001   0.000001-0.327961   0.0       0.0
   K2          0.327961 0.000001  -0.000001 0.327961   0.0       0.0
   LI1         0.012278 0.030996  -0.030996 0.012278   0.0       0.0
   LI2        -0.012278-0.030996   0.030996-0.012278   0.0       0.0
   S1          0.048288-0.178545   0.178545 0.048288   0.0       0.0
   S2         -0.048288 0.178545  -0.178545-0.048288   0.0       0.0
   01          0.108144-0.220869   0.220869 0.108144   0.0       0.0
   05         -0.108144 0.220869  -0.220869-0.108144   0.0       0.0
   02          0.007531-0.091831   0.091103-0.000046  -0.067669 0.098621
   06         -0.007531 0.091831  -0.091103 0.000046  -0.067669 0.098621
   03          0.001533-0.094565   0.088368 0.005952  -0.051574-0.107914
   07         -0.001533 0.094565  -0.088368-0.005952  -0.051574-0.107914
   04          0.002164-0.088004   0.094930 0.005321   0.119243 0.009293
   08         -0.002164 0.088004  -0.094930-0.005321   0.119243 0.009293
NY =   3.88 THZ

   K1          0.338550 0.000001  -0.000001 0.338550   0.0       0.0
   K2         -0.338550-0.000001   0.000001-0.338550   0.0       0.0
   LI1        -0.044613-0.017535   0.017535-0.044613   0.0       0.0
   LI2         0.044613 0.017535  -0.017535 0.044613   0.0       0.0
   S1          0.072718-0.086597   0.086597 0.072718   0.0       0.0
   S2         -0.072718 0.086597  -0.086597-0.072718   0.0       0.0
   01          0.084482-0.245257   0.245257 0.084482   0.0       0.0
   05         -0.084482 0.245257  -0.245257-0.084482   0.0       0.0
   02          0.035520 0.002060  -0.003498 0.035937  -0.040416 0.176459
   06         -0.035520-0.002060   0.003498-0.035937  -0.040416 0.176459
   03          0.035210 0.003319  -0.002239 0.036246  -0.132610-0.123231
   07         -0.035210-0.003319   0.002239-0.036246  -0.132610-0.123231
   04          0.036455 0.002957  -0.002600 0.035001   0.173026-0.053228
   08         -0.036455-0.002957   0.002600-0.035001   0.173026-0.053228
NY =   8.54 THZ

   K1          0.028613 0.000000  -0.000000 0.028613   0.0       0.0
   K2         -0.028613-0.000000   0.000000-0.028613   0.0       0.0
   LI1         0.479262 0.088713  -0.088713 0.479262   0.0       0.0
   LI2        -0.479262-0.088713   0.088713-0.479262   0.0       0.0
   S1          0.036493 0.008705  -0.008705 0.036493   0.0       0.0
   S2         -0.036493-0.008705   0.008705-0.036493   0.0       0.0
   01          0.021423-0.010564   0.010564 0.021423   0.0       0.0
   05         -0.021423 0.010564  -0.010564-0.021423   0.0       0.0
   02          0.044962 0.014089  -0.006052 0.041158   0.045967 0.019066
   06         -0.044962-0.014089   0.006052-0.041158   0.045967 0.019066
   03          0.045589 0.006414  -0.013727 0.040531  -0.039496 0.030276
   07         -0.045589-0.006414   0.013727-0.040531  -0.039496 0.030276
   04          0.038629 0.009709  -0.010432 0.047491  -0.006472-0.049342
   08         -0.038629-0.009708   0.010432-0.047491  -0.006472-0.049342
```

```
 NY =  16.37 THZ

    K1          0.009137 0.000000   -0.000000 0.009137    0.0       0.0
    K2         -0.009137-0.000000    0.000000-0.009137    0.0       0.0
    L11        -0.021813-0.005222    0.005222-0.021813    0.0       0.0
    L12         0.021813 0.005222   -0.005222 0.021813    0.0       0.0
    S1          0.021777 0.033304   -0.033304 0.021777    0.0       0.0
    S2         -0.021777-0.033304    0.033304-0.021777    0.0       0.0
    01          0.208682 0.085933   -0.085933 0.208682    0.0       0.0
    05         -0.208682-0.085933    0.085933-0.208682    0.0       0.0
    02          0.078911 0.030396    0.117033-0.248627    0.203210 0.085482
    06         -0.078911-0.030396   -0.117033 0.248628    0.203210 0.085482
    03         -0.102904-0.222004   -0.135367-0.066812   -0.175635 0.133245
    07          0.102904 0.222004    0.135366 0.066812   -0.175635 0.133245
    04         -0.230582 0.061652    0.148290 0.060865   -0.027576-0.218726
    08          0.230581-0.061653   -0.148290-0.060865   -0.027576-0.218727
 NY =  17.21 THZ

    K1          0.004454 0.000000   -0.000000 0.004454    0.0       0.0
    K2         -0.004454-0.000000    0.000000-0.004454    0.0       0.0
    L11         0.003656-0.018961    0.018961 0.003656    0.0       0.0
    L12        -0.003656 0.018961   -0.018961-0.003656    0.0       0.0
    S1         -0.013687-0.332986    0.332986-0.013687    0.0       0.0
    S2          0.013687 0.332986   -0.332986 0.013687    0.0       0.0
    01          0.031559 0.249599   -0.249599 0.031559    0.0       0.0
    05         -0.031559-0.249599    0.249599-0.031559    0.0       0.0
    02         -0.005853-0.044974   -0.187778 0.003757    0.020034 0.111489
    06          0.005853 0.044974    0.187778-0.003757    0.020034 0.111489
    03         -0.099430 0.133751   -0.009052 0.097334   -0.106570-0.038395
    07          0.099429-0.133751    0.009052-0.097334   -0.106570-0.038395
    04          0.102139 0.125428   -0.017375-0.104235    0.086536-0.073095
    08         -0.102140-0.125428    0.017375 0.104235    0.086536-0.073095
 NY =  34.20 THZ

    K1          0.001921 0.000000   -0.000000 0.001921    0.0       0.0
    K2         -0.001921-0.000000    0.000000-0.001921    0.0       0.0
    L11        -0.000350-0.002747    0.002747-0.000350    0.0       0.0
    L12         0.000350 0.002747   -0.002747 0.000350    0.0       0.0
    S1          0.172465 0.157572   -0.157572 0.172465    0.0       0.0
    S2         -0.172465-0.157572    0.157572-0.172465    0.0       0.0
    01          0.047270 0.040131   -0.040131 0.047270    0.0       0.0
    05         -0.047270-0.040131    0.040131-0.047270    0.0       0.0
    02         -0.248168-0.209454   -0.031558 0.054853    0.102750 0.087706
    06          0.248166 0.209454    0.031559-0.054853    0.102750 0.087706
    03         -0.125264 0.102518    0.280413-0.068052   -0.127331 0.045131
    07          0.125263-0.102517   -0.280413 0.068052   -0.127331 0.045131
    04          0.083459-0.159907    0.017990-0.276775    0.024581-0.132837
    08         -0.083459 0.159907   -0.017988 0.276775    0.024580-0.132838
EIGENVALUES AND EIGENVECTORS FOR IRM  4

 NY =   4.07 THZ

    K1          0.0       0.0       0.0       0.0       -0.262818-0.000003
    K2          0.0       0.0       0.0       0.0        0.262818 0.000003
    L11         0.0       0.0       0.0       0.0       -0.067335-0.000001
    L12         0.0       0.0       0.0       0.0        0.067335 0.000001
    S1          0.0       0.0       0.0       0.0       -0.212086-0.000003
    S2          0.0       0.0       0.0       0.0        0.212086 0.000002
    01          0.0       0.0       0.0       0.0       -0.133194-0.000002
    05          0.0       0.0       0.0       0.0        0.133194 0.000001
    02          0.015701 0.000000   0.325520 0.000005   -0.122535-0.000002
    06          0.015701 0.000000   0.325520 0.000003    0.122535 0.000001
    03         -0.289759-0.000002  -0.149162-0.000001   -0.122535-0.000001
    07         -0.289759-0.000004  -0.149162-0.000002    0.122535 0.000002
    04          0.274058 0.000003  -0.176357-0.000002   -0.122535-0.000002
    08          0.274058 0.000002  -0.176357-0.000002    0.122535 0.000001
 NY =   4.61 THZ

    K1          0.0       0.0       0.0       0.0        0.196349 0.000002
    K2          0.0       0.0       0.0       0.0       -0.196349-0.000002
    L11         0.0       0.0       0.0       0.0        0.015846 0.000000
    L12         0.0       0.0       0.0       0.0       -0.015846-0.000000
    S1          0.0       0.0       0.0       0.0       -0.388628-0.000005
    S2          0.0       0.0       0.0       0.0        0.388628 0.000004
    01          0.0       0.0       0.0       0.0       -0.252514-0.000003
    05          0.0       0.0       0.0       0.0        0.252514 0.000002
    02         -0.002322-0.000000  -0.155427-0.000002   -0.240772-0.000004
    06         -0.002322-0.000000  -0.155427-0.000002    0.240772 0.000002
    03          0.135765 0.000001   0.075703 0.000001   -0.240772-0.000002
    07          0.135765 0.000002   0.075703 0.000001    0.240772 0.000004
    04         -0.133443-0.000002   0.079724 0.000001   -0.240772-0.000003
    08         -0.133443-0.000001   0.079724 0.000001    0.240772 0.000002
 NY =   6.18 THZ

    K1          0.0       0.0       0.0       0.0        0.622533 0.000008
    K2          0.0       0.0       0.0       0.0       -0.622533-0.000006
    L11         0.0       0.0       0.0       0.0        0.043799 0.000001
    L12         0.0       0.0       0.0       0.0       -0.043799-0.000000
    S1          0.0       0.0       0.0       0.0        0.039650 0.000001
    S2          0.0       0.0       0.0       0.0       -0.039650-0.000000
    01          0.0       0.0       0.0       0.0        0.012251 0.000000
    05          0.0       0.0       0.0       0.0       -0.012251-0.000000
    02          0.005847 0.000000   0.189026 0.000003    0.022490 0.000000
    06          0.005847 0.000000   0.189026 0.000002   -0.022490-0.000000
    03         -0.166625-0.000001  -0.089449-0.000001    0.022490 0.000000
    07         -0.166625-0.000002  -0.089449-0.000001   -0.022490-0.000000
    04          0.160778 0.000002  -0.099576-0.000001    0.022490 0.000000
    08          0.160778 0.000001  -0.099576-0.000001   -0.022490-0.000000
```

```
NY =  8.94 THZ

   K1          0.0      0.0         0.0      0.0         0.068170 0.000001
   K2          0.0      0.0         0.0      0.0        -0.068170-0.000001
   LI1         0.0      0.0         0.0      0.0        -0.694225-0.000009
   LI2         0.0      0.0         0.0      0.0         0.694225 0.000007
   S1          0.0      0.0         0.0      0.0        -0.048423-0.000001
   S2          0.0      0.0         0.0      0.0         0.048423 0.000000
   O1          0.0      0.0         0.0      0.0        -0.020921-0.000000
   O5          0.0      0.0         0.0      0.0         0.020921 0.000000
   O2          0.015880 0.000000   -0.024064-0.000000    0.052049 0.000001
   O6          0.015880 0.000000   -0.024064-0.000000   -0.052049-0.000001
   O3          0.012900 0.000000    0.025785 0.000000    0.052049 0.000001
   O7          0.012900 0.000000    0.025785 0.000000   -0.052049-0.000001
   O4         -0.028780-0.000000   -0.001720-0.000000    0.052049 0.000001
   O8         -0.028780-0.000000   -0.001720 0.000000   -0.052049-0.000000
NY = 18.11 THZ

   K1          0.0      0.0         0.0      0.0         0.005405 0.000000
   K2          0.0      0.0         0.0      0.0        -0.005405-0.000000
   LI1         0.0      0.0         0.0      0.0        -0.105381-0.000001
   LI2         0.0      0.0         0.0      0.0         0.105381 0.000001
   S1          0.0      0.0         0.0      0.0         0.438011 0.000006
   S2          0.0      0.0         0.0      0.0        -0.438011-0.000004
   O1          0.0      0.0         0.0      0.0         0.104057 0.000001
   O5          0.0      0.0         0.0      0.0        -0.104057-0.000001
   O2         -0.139086-0.000002    0.006435 0.000000   -0.275697-0.000004
   O6         -0.139086-0.000001    0.006435 0.000000    0.275697 0.000003
   O3          0.063969 0.000001   -0.123669-0.000001   -0.275697-0.000003
   O7          0.063969 0.000001   -0.123669-0.000002    0.275697 0.000004
   O4          0.075116 0.000001    0.117234 0.000001   -0.275697-0.000003
   O8          0.075116 0.000001    0.117234 0.000001    0.275697 0.000002
NY = 33.79 THZ

   K1          0.0      0.0         0.0      0.0         0.010019 0.000000
   K2          0.0      0.0         0.0      0.0        -0.010019-0.000000
   LI1         0.0      0.0         0.0      0.0        -0.008766-0.000000
   LI2         0.0      0.0         0.0      0.0         0.008766 0.000000
   S1          0.0      0.0         0.0      0.0        -0.328605-0.000004
   S2          0.0      0.0         0.0      0.0         0.328605 0.000003
   O1          0.0      0.0         0.0      0.0         0.543507 0.000007
   O5          0.0      0.0         0.0      0.0        -0.543507-0.000005
   O2         -0.178550-0.000003    0.008125 0.000000   -0.014196-0.000000
   O6         -0.178550-0.000002    0.008125 0.000000    0.014196 0.000000
   O3          0.082239 0.000001   -0.158691-0.000001   -0.014196-0.000000
   O7          0.082239 0.000001   -0.158691-0.000002    0.014196 0.000000
   O4          0.096311 0.000001    0.150567 0.000002   -0.014196-0.000000
   O8          0.096311 0.000001    0.150567 0.000001    0.014196 0.000000
NY = 39.51 THZ

   K1          0.0      0.0         0.0      0.0         0.007083 0.000000
   K2          0.0      0.0         0.0      0.0        -0.007083-0.000000
   LI1         0.0      0.0         0.0      0.0        -0.012862-0.000000
   LI2         0.0      0.0         0.0      0.0         0.012862 0.000000
   S1          0.0      0.0         0.0      0.0         0.015380 0.000000
   S2          0.0      0.0         0.0      0.0        -0.015380-0.000000
   O1          0.0      0.0         0.0      0.0         0.334189 0.000004
   O5          0.0      0.0         0.0      0.0        -0.334189-0.000003
   O2          0.338975 0.000005   -0.011356-0.000000   -0.119399-0.000002
   O6          0.338975 0.000003   -0.011356-0.000000    0.119399 0.000001
   O3         -0.159653-0.000002    0.299239 0.000003   -0.119399-0.000001
   O7         -0.159653-0.000002    0.299239 0.000004    0.119399 0.000002
   O4         -0.179321-0.000002   -0.287883-0.000003   -0.119399-0.000001
   O8         -0.179321-0.000002   -0.287883-0.000002    0.119399 0.000001

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*********  Q = ( 0.0 , 0.0 , 0.07) 1/A **********  QHKL = ( 0.0 , 0.0 , 0.10)  **********


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EIGENVALUES AND EIGENVECTORS FOR IRM  1

NY =  0.59 THZ

   K1          0.0      0.0         0.0      0.0         0.370235 0.000001
   K2          0.0      0.0         0.0      0.0         0.352114 0.114408
   LI1         0.0      0.0         0.0      0.0         0.148278 0.045695
   LI2         0.0      0.0         0.0      0.0         0.155141-0.002362
   S1          0.0      0.0         0.0      0.0         0.332385 0.054072
   S2          0.0      0.0         0.0      0.0         0.299408 0.154137
   O1          0.0      0.0         0.0      0.0        -0.234280 0.039075
   O5          0.0      0.0         0.0      0.0         0.210739 0.109558
   O2         -0.000065-0.000122   -0.001304 0.001310    0.234559 0.036391
   O6          0.000024 0.000136    0.001645-0.000843    0.211835 0.107091

                                    .
                                    .
                                    .
```

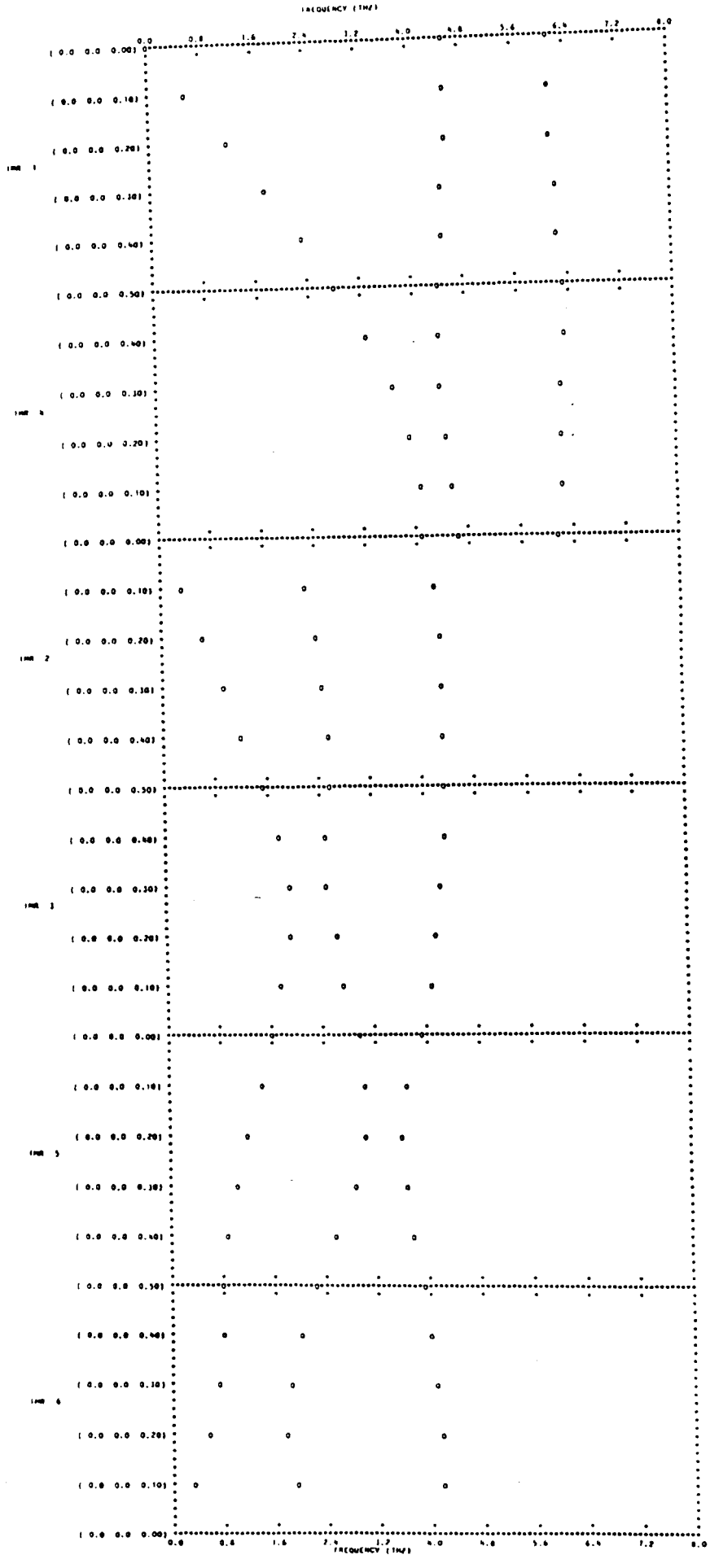
A.5 HIST

INPUT

```
6.5
    1   -4    2   -3    5   -6    0
    3
```

OUTPUT

The heading is the same as for **MODEL1**.



A.6 SF

INPUT

```
    0     3     0     3     0     3
5.0
0.35       -0.18       0.31        0.577       0.577
     1    0.0174      0.000       0.000       0.0174      0.000      0.0174
     3    0.0201      0.000       0.000       0.0201      0.000      0.0201
     5    0.0084      0.000       0.000       0.0084      0.000      0.0084
     7    0.0218      0.000       0.000       0.0218      0.000      0.0218
     9  0.001420    0.001010    0.000970    0.002050   -0.00220    0.005070
298.
10000.
     1     0     0     0     0     0     0     0     0     0
```

OUTPUT

```
LATTICE DYNAMICAL MODEL-CALCULATION FOR THE FOLLOWING STRUCTURE:
-----------------------------------------------------------------------------------------------------------

 POSITION VECTOR SPACE LATTICE VECTORS
A 1 = (  5.14200,  0.0     ,  0.0     )
A 2 = ( -2.57100,  4.45300,  0.0     )
A 3 = (  0.0     ,  0.0     ,  8.62400)

AI 1 = (  0.19448,  0.11228,  0.0     )
AI 2 = (  0.0     ,  0.22457,  0.0     )
AI 3 = (  0.0     ,  0.0     ,  0.11595)
 RECIPROCAL SPACE LATTICE VECTORS

        14 PARTICLES PER UNIT CELL
                                POSITION                          MASS   SCATT. LENGTH   TENSOR OF TEMP.FACTORS

        K1      (  0.0     ,  0.0     ,  0.0     )              39.10       0.35        0.01740   0.0       0.0
                                                                                        0.0       0.01740   0.0
                                                                                        0.0       0.0       0.01740
        K2      (  0.0     ,  0.0     ,  4.31200)              39.10       0.35        0.01740   0.0       0.0
                                                                                        0.0       0.01740   0.0
                                                                                        0.0       0.0       0.01740
        LI1     (  0.0     ,  2.96874,  5.88200)               6.94      -0.18        0.02010   0.0       0.0
                                                                                        0.0       0.02010   0.0
                                                                                        0.0       0.0       0.02010
        LI2     (  2.57100,  1.48437,  1.57000)               6.94      -0.18        0.02010   0.0       0.0
                                                                                        0.0       0.02010   0.0
                                                                                        0.0       0.0       0.02010
        S1      (  0.0     ,  2.96874,  2.53500)              32.06       0.31        0.00840   0.0       0.0
                                                                                        0.0       0.00840   0.0
                                                                                        0.0       0.0       0.00840
        S2      (  2.57100,  1.48437,  6.84700)              32.06       0.31        0.00840  -0.00000   0.0
                                                                                        0.00000   0.00840   0.0
                                                                                        0.0       0.0       0.00840
        O1      (  0.0     ,  2.96870,  3.96700)              16.00       0.58        0.02180   0.0       0.0
                                                                                        0.0       0.02180   0.0
                                                                                        0.0       0.0       0.02180
        O5      (  2.57100,  1.48440,  8.27900)              16.00       0.58        0.02180   0.0       0.0
                                                                                        0.0       0.02180   0.0
                                                                                        0.0       0.0       0.02180
        O2      (  1.39090,  2.92570,  2.06110)              16.00       0.58        0.00142   0.00101   0.00097
                                                                                        0.00101   0.00205  -0.00220
                                                                                        0.00097  -0.00220   0.00507
        O6      (  1.18010,  1.52740,  6.37310)              16.00       0.58        0.00142   0.00101  -0.00097
                                                                                        0.00101   0.00205   0.00220
                                                                                       -0.00097   0.00220   0.00507
        O3      (  4.48380,  4.19480,  2.06110)              16.00       0.58        0.00102  -0.00078  -0.00239
                                                                                       -0.00078   0.00245   0.00026
                                                                                       -0.00239   0.00026   0.00507
        O7      (  3.22920,  0.25830,  6.37310)              16.00       0.58        0.00102  -0.00078   0.00239
                                                                                       -0.00078   0.00245  -0.00026
                                                                                        0.00239  -0.00026   0.00507
        O4      (  4.40930,  1.78570,  2.06110)              16.00       0.58        0.00277  -0.00023   0.00142
                                                                                       -0.00023   0.00070   0.00194
                                                                                        0.00142   0.00194   0.00507
        O8      (  3.30370,  2.66740,  6.37310)              16.00       0.58        0.00277  -0.00023  -0.00142
                                                                                       -0.00023   0.00070  -0.00194
                                                                                       -0.00142  -0.00194   0.00507
-----------------------------------------------------------------------------------------------------------

MODEL SPECIFICATIONS :

        INTERACTION             TYPE            NEIGHBOR    PARAMETER-NO.S

        K1   - K1       COULOMB (M-M)            **          Z1   =  1   Z2   =  1

                                .
                                .
                                .
```

********** Q = (0.0 , 0.0 , 0.00) 1/A ********** QHKL = (0.0 , 0.0 , 0.00) **********

1	0.0	4.59	6.17	9.79	18.04	33.79	39.57
2	0.0	2.07	4.23	8.60	16.51	17.15	34.21
2	0.0	2.07	4.23	8.60	16.51	17.15	34.21
3	1.62	2.93	3.88	8.54	16.37	17.21	34.20
3	1.62	2.93	3.88	8.54	16.37	17.21	34.20
4	4.07	4.61	6.18	8.94	18.11	33.79	39.51

0 0 1	0.	0.	0.	0.	0.	0.	0.
	0.	0.	0.	0.	0.	0.	0.
	0.	0.	0.	0.	0.	0.	0.
	0.	0.	0.	0.	0.	0.	0.
	0.	0.	0.	0.	0.	0.	0.
	113.	415.	30.	14.	228.	107.	87.
0 0 2	339.	23.	307.	387.	1403.	656.	795.
	0.	0.	0.	0.	0.	0.	0.
	0.	0.	0.	0.	0.	0.	0.
	0.	0.	0.	0.	0.	0.	0.
	0.	0.	0.	0.	0.	0.	0.
	0.	0.	0.	0.	0.	0.	0.
0 0 3	0.	0.	0.	0.	0.	0.	0.
	0.	0.	0.	0.	0.	0.	0.
	0.	0.	0.	0.	0.	0.	0.
	0.	0.	0.	0.	0.	0.	0.
	0.	0.	0.	0.	0.	0.	0.
	442.	1893.	182.	362.	2639.	1714.	1337.
0 1 0	0.	237.	25.	0.	20.	33.	114.
	9.	7.	144.	43.	124.	88.	174.
	9.	7.	144.	43.	124.	88.	174.
	47.	176.	116.	36.	34.	136.	130.
	47.	176.	116.	36.	34.	136.	130.
	51.	14.	19.	2.	76.	125.	446.
0 1 1	71.	75.	41.	14.	37.	7.	729.
	134.	2.	55.	50.	528.	65.	30.
	134.	19.	50.	51.	51.	276.	283.
	10.	3.	135.	20.	469.	2.	61.
	33.	41.	75.	45.	7.	194.	306.
	94.	75.	157.	10.	8.	0.	202.
0 1 2	70.	269.	101.	15.	18.	167.	241.
	33.	392.	75.	21.	17.	110.	383.
	33.	75.	17.	22.	782.	47.	33.
	362.	64.	204.	77.	221.	121.	380.
	172.	19.	47.	129.	976.	62.	21.
	128.	12.	11.	147.	42.	509.	817.
0 1 3	124.	137.	50.	166.	131.	1908.	219.
	26.	1203.	129.	58.	800.	79.	46.
	26.	1584.	75.	40.	80.	48.	500.
	258.	119.	250.	2.	783.	117.	39.
	522.	199.	219.	28.	36.	89.	476.
	450.	85.	66.	52.	52.	621.	73.
0 2 0	0.	2985.	289.	3.	4.	9.	26.
	82.	200.	234.	67.	14.	93.	797.
	82.	200.	234.	67.	14.	93.	797.
	56.	263.	356.	250.	27.	431.	1988.
	56.	263.	356.	250.	28.	431.	1988.
	569.	133.	195.	5.	21.	35.	118.
0 2 1	18.	851.	51.	45.	109.	190.	35.
	135.	405.	152.	264.	499.	120.	1845.
	135.	596.	121.	325.	381.	310.	1556.
	11.	208.	295.	54.	161.	42.	924.
	485.	244.	115.	33.	216.	113.	495.
	2410.	416.	470.	35.	41.	52.	9.
0 2 2	42.	2893.	543.	16.	113.	149.	14.
	79.	383.	345.	38.	929.	354.	203.
	79.	529.	588.	38.	42.	11.	1031.
	90.	193.	177.	381.	1605.	182.	954.
	40.	498.	530.	260.	599.	31.	1612.
	427.	419.	220.	146.	181.	460.	92.
0 2 3	169.	673.	222.	296.	244.	726.	609.
	141.	366.	139.	249.	207.	859.	1850.
	141.	210.	79.	249.	1895.	524.	736.
	62.	195.	1044.	150.	164.	343.	1379.
	686.	21.	627.	123.	1515.	309.	79.
	1429.	537.	1603.	129.	170.	267.	160.
0 3 0	0.	161.	30.	5.	723.	1201.	4171.
	4527.	36.	488.	1709.	197.	1073.	26.
	4527.	36.	488.	1709.	197.	1073.	26.
	5.	0.	0.	0.	1226.	516.	1409.
	5.	0.	0.	0.	1226.	516.	1409.
	574.	129.	192.	2.	4.	6.	24.
0 3 1	0.	814.	79.	1.	4.	7.	23.
	4.	21.	2.	0.	1418.	324.	1377.
	4.	8.	2.	0.	1369.	385.	1437.
	1591.	3593.	434.	1068.	906.	490.	99.
	2387.	1055.	1884.	1237.	1201.	423.	13.
	199.	149.	110.	17.	937.	1801.	3509.
0 3 2	86.	118.	252.	200.	1506.	1853.	3961.
	363.	1625.	440.	696.	2693.	610.	191.
	363.	3410.	1340.	684.	2407.	228.	127.
	9.	11.	25.	2.	1263.	520.	1464.
	51.	7.	19.	2.	1229.	516.	1347.
	566.	130.	190.	2.	5.	6.	24.

A.7 PARDER

INPUT

```
    0    0    0    0    0    0    0    0    0    0
.01      .01      .01      .01      .01      .001     .001     .001
.001     50.      5.0      1.0      5.0      1.0      10.0     1.0
10.0     1.0
```

OUTPUT

The heading is the same as for **MODEL1**.

```
MESSAGE FOR Q = ( 0.0 , 0.0 , 0.0 ) 1/A :
***  PARTIAL-DERIVATIVE OF FREQUENCY NO.  1 WITH RESPECT TO PARAMETER NO.  3 IS DERIVATIVE OF NY**2
***  PARTIAL-DERIVATIVE OF FREQUENCY NO.  1 WITH RESPECT TO PARAMETER NO. 11 IS DERIVATIVE OF NY**2
***  PARTIAL-DERIVATIVE OF FREQUENCY NO.  1 WITH RESPECT TO PARAMETER NO. 12 IS DERIVATIVE OF NY**2
***  PARTIAL-DERIVATIVE OF FREQUENCY NO.  1 WITH RESPECT TO PARAMETER NO. 18 IS DERIVATIVE OF NY**2
-------------------------------------------------------------------------------------------------------------------------------

*********  Q  =  ( 0.0 , 0.0 , 0.00) 1/A **********  QHKL  =  ( 0.0 , 0.0 , 0.00)  **********


-------------------------------------------------------------------------------------------------------------------------------
THE FREQUENCY-SHIFTS ARE CALCULATED WITH RESPECT TO THE FOLLOWING PARAMETER-VARIATIONS:

                0.0100 0.0100 0.0100 0.0100 0.0100 0.0010 0.0010 0.0010 0.001050.0000 5.0000 1.0000 5.0000 1.000010.0000
                1.000010.0000 1.0000
PARTIAL DERIVATIVES IN THZ/DP FOR IRM  1

NY =  0.0  THZ     0.008  0.006 -0.000  0.007  0.004  0.006  0.004  0.0 06  0.003  0.006 -0.000 -0.000  0.006  0.006  0.007
                   0.006  0.003 -0.000
NY =  4.59 THZ    -0.006 -0.017  0.041  0.004 -0.065  0.022  0.049  0.0 04  0.066  0.048  0.000  0.094  0.000  0.283  0.000
                   0.000  0.000  0.094
NY =  6.17 THZ    -0.001 -0.021 -0.007 -0.014 -0.021  0.057  0.026  0.0 11  0.072  0.072  0.000  0.007  0.000  0.020  0.001
                  -0.000  0.000  0.008
NY =  9.79 THZ    -0.007  0.000 -0.012  0.019 -0.061  0.004  0.176  0.1 86 -0.007  0.111  0.000  0.000  0.001  0.000  0.004
                  -0.000  0.001  0.002
NY = 18.04 THZ     0.000  0.009  0.032  0.006 -0.077  0.009 -0.004 -0.0 00  0.005  0.006  0.044  0.019  0.047 -0.000  0.018
                  -0.000  0.005  0.056
NY = 33.79 THZ     0.002 -0.004 -0.024  0.032  0.006 -0.001  0.017  0.0 15  0.002  0.009  0.047  0.018  0.041  0.000  0.168
                   0.000  0.050  0.002
NY = 39.57 THZ     0.001 -0.002 -0.013 -0.000  0.000  0.001  0.010  0.0 04  0.007  0.007  0.117  0.000  0.123  0.000  0.027
                   0.000  0.093  0.000
```

```
PARTIAL DERIVATIVES IN THZ/DP FOR IRM  2
(2-FOLD DEGENERATE)
NY =  0.0  THZ      0.006  0.007  0.009  0.007  0.010  0.007  0.007  0.0 07  0.007  0.006  0.007  0.007  0.007  0.007  0.007
                    0.006  0.008  0.009
NY =  2.07 THZ     -0.001  0.058  0.130 -0.009  0.069  0.093 -0.026  0.0 16  0.050  0.076  0.000  0.528  0.000  0.338  0.000
                    0.076  0.000  0.141
NY =  4.23 THZ     -0.009  0.008  0.011  0.018  0.013  0.082 -0.001  0.0 49  0.032  0.082  0.000  0.016  0.000  0.009  0.000
                    0.003  0.000  0.004
NY =  8.60 THZ      0.006 -0.002  0.006 -0.012  0.038  0.000  0.195 -0.0 26  0.221  0.109  0.000  0.000  0.000  0.000  0.000
                    0.000  0.000  0.000
NY = 16.51 THZ     -0.001  0.000  0.015 -0.001 -0.022  0.010  0.008  0.0 02  0.016  0.015  0.046  0.042  0.095  0.041  0.000
                    0.003  0.002  0.028
NY = 17.15 THZ     -0.000  0.002  0.028 -0.028 -0.022  0.008  0.003  0.0 03  0.007  0.009  0.071  0.007  0.023  0.014  0.000
                    0.028  0.034  0.032
NY = 34.21 THZ      0.000 -0.001 -0.022 -0.003  0.039  0.002  0.006  0.0 00  0.008  0.006  0.048  0.005  0.047  0.014  0.000
                    0.001  0.214  0.001
NY =  0.0  THZ      0.006  0.007  0.009  0.007  0.010  0.007  0.007  0.0 07  0.007  0.006  0.007  0.007  0.007  0.007  0.007
                    0.006  0.008  0.009
NY =  2.07 THZ     -0.001  0.058  0.130 -0.009  0.069  0.093 -0.026  0.0 16  0.050  0.076  0.000  0.528  0.000  0.338  0.000
                    0.076  0.000  0.141
NY =  4.23 THZ     -0.009  0.008  0.011  0.018  0.013  0.082 -0.001  0.0 49  0.032  0.082  0.000  0.016  0.000  0.009  0.000
                    0.003  0.000  0.004
NY =  8.60 THZ      0.006 -0.002  0.006 -0.012  0.038  0.000  0.195 -0.0 26  0.221  0.109  0.000  0.000  0.000  0.000  0.000
                    0.000  0.000  0.000
NY = 16.51 THZ     -0.001  0.000  0.015 -0.001 -0.022  0.010  0.008  0.0 02  0.016  0.015  0.046  0.042  0.095  0.041  0.000
                    0.003  0.002  0.028
NY = 17.15 THZ     -0.000  0.002  0.028 -0.028 -0.022  0.008  0.003  0.0 03  0.007  0.009  0.071  0.007  0.023  0.014  0.000
                    0.028  0.034  0.032
NY = 34.21 THZ      0.000 -0.001 -0.022 -0.003  0.039  0.002  0.006  0.0 00  0.008  0.006  0.048  0.005  0.047  0.014  0.000
                    0.001  0.214  0.001
PARTIAL DERIVATIVES IN THZ/DP FOR IRM  3
(2-FOLD DEGENERATE)
NY =  1.62 THZ      0.009  0.030  0.079 -0.003  0.031  0.028 -0.008  0.0 13  0.006  0.025  0.000  0.304  0.000  0.197  0.000
                    0.043  0.000  0.083
NY =  2.93 THZ     -0.004  0.018  0.020 -0.000  0.008  0.041 -0.006  0.0 14  0.021  0.038  0.000  0.068  0.000  0.042  0.000
                    0.009  0.000  0.018
NY =  3.88 THZ     -0.013  0.018  0.031  0.005  0.020  0.092 -0.008  0.0 39  0.044  0.084  0.000  0.118  0.000  0.072  0.000
                    0.017  0.000 -0.030
NY =  8.54 THZ      0.006 -0.004  0.007 -0.010  0.037  0.001  0.196 -0.0 22  0.219  0.111  0.001  0.001  0.000  0.003  0.000
                    0.000  0.000  0.001
NY = 16.37 THZ     -0.001  0.001  0.015 -0.001 -0.015  0.012  0.009  0.0 02  0.018  0.016  0.059  0.044  0.084  0.042  0.000
                    0.005  0.000  0.025
NY = 17.21 THZ     -0.001  0.002  0.029 -0.027 -0.025  0.007  0.002  0.0 03  0.007  0.008  0.059  0.006  0.034  0.013  0.000
                    0.026  0.034  0.034
NY = 34.20 THZ      0.000 -0.001 -0.022 -0.003  0.039  0.002  0.006  0.0 00  0.008  0.006  0.047  0.005  0.047  0.014  0.000
                    0.001  0.214  0.001
NY =  1.62 THZ      0.009  0.030  0.079 -0.003  0.031  0.028 -0.008  0.0 13  0.006  0.025  0.000  0.304  0.000  0.197  0.000
                    0.043  0.000  0.083
NY =  2.93 THZ     -0.004  0.018  0.020 -0.000  0.008  0.041 -0.006  0.0 14  0.021  0.038  0.000  0.068  0.000  0.042  0.000
                    0.009  0.000  0.018
NY =  3.88 THZ     -0.013  0.018  0.031  0.005  0.020  0.092 -0.008  0.0 39  0.044  0.084  0.000  0.118  0.000  0.072  0.000
                    0.017  0.000  0.030
NY =  8.54 THZ      0.006 -0.004  0.007 -0.010  0.037  0.001  0.196 -0.0 22  0.219  0.111  0.001  0.001  0.000  0.003  0.000
                    0.000  0.000  0.001
NY = 16.37 THZ     -0.001  0.001  0.015 -0.001 -0.015  0.012  0.009  0.0 02  0.018  0.016  0.059  0.044  0.084  0.042  0.000
                    0.005  0.000  0.025
NY = 17.21 THZ     -0.001  0.002  0.029 -0.027 -0.025  0.007  0.002  0.0 03  0.007  0.008  0.059  0.006  0.034  0.013  0.000
                    0.026  0.034  0.034
NY = 34.20 THZ      0.000 -0.001 -0.022 -0.003  0.039  0.002  0.006  0.0 00  0.008  0.006  0.047  0.005  0.047  0.014  0.000
                    0.001  0.214  0.001
PARTIAL DERIVATIVES IN THZ/DP FOR IRM  4

NY =  4.07 THZ      0.005 -0.001  0.028 -0.001 -0.068 -0.003  0.017 -0.0 03  0.016  0.009  0.000  0.074  0.000  0.222  0.001
                   -0.000  0.000  0.075
NY =  4.61 THZ      0.003 -0.010  0.004 -0.001 -0.024  0.015  0.047  0.0 26  0.036  0.042  0.000  0.015  0.000  0.045  0.001
                    0.000  0.000  0.016
NY =  6.18 THZ     -0.001 -0.013  0.001 -0.011 -0.007  0.076  0.015 -0.0 03  0.095  0.082  0.000  0.016 -0.000  0.049  0.000
                   -0.000 -0.000  0.016
NY =  8.94 THZ     -0.010 -0.013 -0.010  0.020 -0.062  0.001  0.185  0.1 93 -0.008  0.113  0.004  0.001  0.001  0.000  0.000
                   -0.000  0.000  0.003
NY = 18.11 THZ     -0.000  0.010  0.031  0.006 -0.079  0.006  0.002  0.0 06  0.001  0.007  0.040  0.018  0.046  0.000  0.022
                    0.000  0.005  0.056
NY = 33.79 THZ      0.002 -0.004 -0.024  0.032  0.004 -0.001  0.016  0.0 14  0.001  0.009  0.050  0.019  0.040  0.000  0.169
                    0.000  0.048  0.002
NY = 39.51 THZ      0.001 -0.002 -0.013  0.000  0.001  0.001  0.011  0.0 05  0.007  0.007  0.115  0.000  0.124  0.000  0.025
                    0.000  0.095  0.000
```

A.8 ROTINV

INPUT

```
0.0200
    0     0     0     0     0     0     0     0     0
39.10      6.940       32.06       16.00       16.00
    1
    5     7     1
   15    16
    5     9     1
   17    18
    7     9     1
   11    12
    9    11     1
   13    14
    0
    2
    6     7     7     8     9    10
    1     8     1
    1     9     1
    1    10     1
    3     7     1
    3    10     1
    0
    5
     7.
    1     2     3     4     5
    0
1.20        0.400       1.35        -0.850      -0.700      .197        0.08600     .1060
.100        2000.       125.0       -.5000      125.0       -.300       870.00      -53.8
870.        -38.6
1.10        0.500       1.35        -0.850      -0.700      .197        0.08600     .1060
.100        2000.       125.0       0.0000      125.0       0.000       870.00      -53.8
870.        -38.6
```

OUTPUT

```
NEW PARAMETERVECTOR :

     1.100     0.500     1.350    -0.850    -0.700     0.197     0.086
     0.106     0.100  2000.000   125.000     0.0     125.000     0.0
   870.000   -53.800   870.000   -38.600
```

ATOM	AXIS OF ROTATION	FORCE IN 10**-10 N		
K1	1	(0.000	0.886	0.002)
	2	(-0.888	-0.000	0.001)
	3	(-0.008	-0.001	-0.000)
K2	1	(-0.000	0.886	-0.002)
	2	(-0.888	-0.000	-0.000)
	3	(0.006	0.000	0.000)
LI1	1	(0.002	1.041	0.001)
	2	(-1.043	-0.002	-0.001)
	3	(0.003	0.005	-0.000)
LI2	1	(-0.001	1.042	-0.002)
	2	(-1.040	0.001	0.002)
	3	(-0.002	-0.004	-0.000)
S1	1	(0.001	-0.663	0.006)
	2	(0.663	-0.002	0.009)
	3	(0.007	-0.045	0.001)
S2	1	(-0.005	-0.660	-0.004)
	2	(0.664	0.003	-0.012)
	3	(-0.008	0.043	0.001)
O1	1	(-0.003	-0.389	0.002)
	2	(0.390	0.001	0.011)
	3	(-0.007	-0.005	0.002)
O5	1	(0.001	-0.389	-0.002)
	2	(0.390	-0.003	-0.013)
	3	(0.005	0.005	0.002)

O2	1	(	-0.001	-0.286	-2.838)
	2	(	0.308	-0.000	0.709)
	3	(	2.848	-0.676	0.001)
O6	1	(	-0.001	-0.292	2.841)
	2	(	0.314	0.000	-0.710)
	3	(	-2.848	0.676	0.001)
O3	1	(	0.004	-0.299	0.787)
	2	(	0.287	0.008	-2.824)
	3	(	-0.795	2.822	-0.012)
O7	1	(	0.007	-0.291	-0.790)
	2	(	0.281	0.006	2.826)
	3	(	0.797	-2.820	-0.013)
O4	1	(	-0.004	-0.291	2.048)
	2	(	0.278	-0.004	2.089)
	3	(	-2.049	-2.091	0.008)
O8	1	(	0.000	-0.294	-2.049)
	2	(	0.285	-0.008	-2.087)
	3	(	2.051	2.092	0.008)

NEW PARAMETERVECTOR :

1.200	0.400	1.350	-0.850	-0.700	0.197	0.086
0.106	0.100	2000.000	125.000	-0.500	125.000	-0.300
870.000	-53.800	870.000	-38.600			

ATOM	AXIS OF ROTATION	FORCE IN 10**-10 N			
K1	1	(	0.000	-0.072	0.002)
	2	(	0.069	-0.000	0.001)
	3	(	-0.007	-0.001	-0.000)
K2	1	(	-0.000	-0.072	-0.002)
	2	(	0.069	-0.000	0.000)
	3	(	0.006	0.001	0.000)
LI1	1	(	0.002	-0.101	0.001)
	2	(	0.100	-0.002	-0.001)
	3	(	0.003	0.004	-0.000)
LI2	1	(	-0.001	-0.101	-0.002)
	2	(	0.102	0.001	0.001)
	3	(	-0.002	-0.004	-0.000)
S1	1	(	0.001	0.176	0.006)
	2	(	-0.176	-0.003	0.009)
	3	(	0.006	-0.045	0.002)
S2	1	(	-0.005	0.180	-0.005)
	2	(	-0.175	0.004	-0.012)
	3	(	-0.007	0.042	0.002)
O1	1	(	-0.003	0.195	0.001)
	2	(	-0.193	0.001	0.011)
	3	(	-0.007	-0.005	0.002)
O5	1	(	0.001	0.194	-0.001)
	2	(	-0.193	-0.003	-0.013)
	3	(	0.005	0.005	0.002)
O2	1	(	-0.002	-0.061	0.032)
	2	(	0.082	-0.000	-0.084)
	3	(	-0.020	0.117	0.002)
O6	1	(	-0.001	-0.066	-0.028)
	2	(	0.088	0.000	0.083)
	3	(	0.020	-0.117	0.001)
O3	1	(	0.004	-0.074	0.038)
	2	(	0.062	0.008	0.057)
	3	(	-0.048	-0.060	-0.012)
O7	1	(	0.008	-0.065	-0.041)
	2	(	0.055	0.006	-0.055)
	3	(	0.050	0.062	-0.014)
O4	1	(	-0.004	-0.065	-0.072)
	2	(	0.052	-0.004	0.002)
	3	(	0.073	-0.003	0.008)
O8	1	(	0.001	-0.069	0.071)
	2	(	0.059	-0.009	0.001)
	3	(	-0.071	0.004	0.008)

A.9 EFG

INPUT

```
     1     0     0     0     0     0     0     0     0     0
1.2          0.4          1.35         -0.85        -0.70
7.0
```

OUTPUT

FORCES DUE TO INTERACTION BETWEEN EACH OF THE SUBLATTICES OF UNIT CHARGES IN 10**-10 N

	K1	LI1	S1	O1	O2
K1	0.000	0.000	0.000	0.000	0.000
	0.000	0.001	0.000	0.001	0.001
	-0.000	-5.396	3.729	3.654	-5.547
LI1	0.000	-0.000	0.000	0.000	-0.004
	0.000	-0.000	-0.001	0.001	-0.006
	5.396	0.000	-2.498	44.150	-36.713
S1	-0.000	0.000	0.000	0.000	0.000
	0.000	-0.001	-0.000	0.003	0.002
	-3.728	2.498	-0.000	-98.427	91.254
O1	-0.000	0.000	0.000	-0.000	-0.001
	0.001	-0.001	-0.003	-0.000	-0.000
	-3.653	-44.150	98.427	-0.000	39.957
O2	-8.810	-25.291	86.817	11.635	28.099
	-10.616	31.232	-2.033	3.580	0.676
	1.849	12.237	-30.418	-13.319	-0.001

						ELECTRICAL FIELD IN V/A			ELECTRICAL FIELD GRADIENT IN V/A**2		
K1	CHARGE = 1.20 AT (	0.0	0.0	0.0) :	(	-0.00000	-0.00003	0.22821)	-0.06105	0.00003	0.0
									0.00003	-0.06120	0.00003
									0.0	0.00003	0.12231
K2	CHARGE = 1.20 AT (	0.0	0.0	4.312) :	(	0.00000	0.00000	0.22824)	-0.06097	0.00002	0.00000
									0.00002	-0.06112	-0.00005
									0.00000	-0.00005	0.12228
LI1	CHARGE = 0.40 AT (	0.0	2.969	5.882) :	(	0.00016	0.00017	-0.54537)	-0.15979	0.00024	0.00012
									0.00024	-0.15942	0.00028
									0.00012	0.00028	0.31925
LI2	CHARGE = 0.40 AT (	2.571	1.484	1.570) :	(	-0.00016	-0.00021	-0.54534)	-0.15953	0.00018	-0.00012
									0.00018	-0.15938	-0.00022
									-0.00012	-0.00022	0.31929
S1	CHARGE = 1.35 AT (	0.0	2.969	2.535) :	(	-0.00002	-0.00025	1.01937)	-0.92635	-0.00013	0.00004
									-0.00013	-0.92633	-0.00026
									0.00004	-0.00026	1.85302
S2	CHARGE = 1.35 AT (	2.571	1.484	6.847) :	(	0.00001	0.00021	1.01936)	-0.92628	0.00009	-0.00004
									0.00009	-0.92649	0.00007
									-0.00004	0.00007	1.85296
O1	CHARGE = -0.85 AT (	0.0	2.969	3.967) :	(	0.00002	-0.00023	5.17892)	5.39008	0.00001	0.00002
									0.00001	5.39005	0.00055
									0.00002	0.00055	-10.78013
O5	CHARGE = -0.85 AT (	2.571	1.484	8.279) :	(	-0.00002	0.00012	5.17882)	5.39028	0.00001	-0.00002
									0.00001	5.39005	-0.00042
									-0.00002	-0.00042	-10.78019
O2	CHARGE = -0.70 AT (	1.391	2.926	2.061) :	(	4.18469	-0.40673	-1.41435)	-8.10557	0.36394	4.58665
									0.36394	4.72201	-0.18960
									4.58665	-0.18960	3.38340
O6	CHARGE = -0.70 AT (	1.180	1.527	6.373) :	(	-4.18484	0.40661	-1.41439)	-8.10560	0.36382	-4.58665
									0.36382	4.72192	0.18955
									-4.58665	0.18955	3.38347
O3	CHARGE = -0.70 AT (	4.484	4.195	2.061) :	(	-1.74039	3.82739	-1.41438)	1.82993	5.37240	-2.12923
									5.37240	-5.21347	4.06701
									-2.12923	4.06701	3.38352
O7	CHARGE = -0.70 AT (	3.229	0.258	6.373) :	(	1.74036	-3.82724	-1.41433)	1.82998	5.37231	2.12916
									5.37231	-5.21347	-4.06691
									2.12916	-4.06691	3.38345
O4	CHARGE = -0.70 AT (	4.409	1.786	2.061) :	(	-2.44442	-3.42094	-1.41433)	1.20011	-5.73625	-2.45744
									-5.73625	-4.58377	-3.87746
									-2.45744	-3.87746	3.38360
O8	CHARGE = -0.70 AT (	3.304	2.667	6.373) :	(	2.44457	3.42092	-1.41438)	1.20017	-5.73640	2.45750
									-5.73640	-4.58373	3.87760
									2.45750	3.87760	3.38345

Appendix B. Comprehensive List of Input Cards

B.1 Input for Program GROUP

Card 1	**Comment**	[18A4]
Card 2	NA, IPM, IDC, NCC, NX	[5I5]
Card 3	(NAME(I), I = 1,NA)	[18A4]
Card 4	**Comment**	[33A4]
Card 5	((A(I,J), I = 1,3), J = 1,3)	[9F8.5]

For each of the NA + NX atoms one card of the following type must be given:

Card 6	TY, (X(I), I = 1,3), JM	[I5,3F10.5,I5]
Card 7	(QS(I), I = 1,3)	[3F10.5]
Card 8	NIR, IT	[2I5]
Card 9	**Comment**	[18A4]
Card 10	(Q(I), I = 1,3)	[3F10.5]

B.2 Input for Program NN

Card 1	(IDIR(I), I = 1,3)	[3I5]
Card 2	NNS	[I5]
Card 3	DELTA, DMAX	[2F10.6]

B.3 Input for Program MODEL1

Card 1 (IDIR(I), I = 1,10) [10I5]

Card 2 (MASS(I), I = 1,MAXTYP) [8F10.5]

Card 3 N [I5]

For Coulomb interaction only:
Card 4 DMAX [F10.5]

Only for interaction types containing atom-specific or general parameters (see table 1)
Card 5 ((IASP(I,J), J = 1,MAXTYP), I = 1,NASP)
(IGP(K), K = 1,NGP) [16I5]

Not for Coulomb interaction:
Card 6 I J NS [3I5]

If interaction N contains interaction-specific parameters (see the table 1) for each of the NS shells a card of the following type must be given:
Card 7 (IISP(I), I = 1,NISP) [16I5]

Further cards of type 6 and 7.
The end of input for the interaction N ($N \neq 5$) is indicated by a card of type 6 with I = 0.

Further interactions may be specified by repeating the input 3.-7. The end of the model set-up is indicated by a card of type 3 with N = 0.

Card 8 (P(I), I = 1,NP) [8F10.5]

B.4 Input for Program HIST

Card 1 NYMAX [F10.6]

Card 2 (IDIR(I), I = 1,20) [16I5]

Card 3 NMARK [I5]

B.5 Input for Program SF

Card 1 HMIN, HMAX, KMIN, KMAX, LMIN, LMAX [6I5]

Card 2 QMAX [F10.6]

Card 3 (B(I), I = 1,MAXTYP) [8F10.6]

For each of the MAXTYP types of particles a card of the following type must be given:
Card 4 I, (TF(K), K = 1,6) [I5,6F10.6]

Card 5 T [F10.6]

Card 6 FNORM [F10.6]

Card 7 (IDIR(I), I = 1,10) [10I5]

B.6 Input for Program PARDER

Card 1 **(IDIR(I), I = 1,10)** **[10I5]**

Card 2 **(DP(I), I = 1,NP)** **[8F10.6]**

B.7 Input for Program ROTINV

Card 1 **QL** **[F10.6]**

Card 2 **(IDIR(I), I = 1,10)** **[10I5]**

Card 3 **(MASS(I), I = 1,MAXTYP)** **[8F10.5]**

Card 4 **N** **[I5]**

For Coulomb interaction only:
Card 5 **DMAX** **[F10.5]**

Only for interaction types containing atom-specific or general parameters (see table 1)
Card 6 **((IASP(I,J), J = 1,MAXTYP), I = 1,NASP)**
(IGP(K), K = 1,NGP) **[16I5]**

Not for Coulomb interaction:
Card 7 **I J NS** **[3I5]**

If interaction N contains interaction-specific parameters (see the table 1) for each of the NS shells a card of the following type must be given:
Card 8 **(IISP(I), I = 1,NISP)** **[16I5]**

Further cards of type 7 and 8.
The end of input for the interaction N ($N \neq 5$) is indicated by a card of type 7 with I = 0.
Further interactions may be specified by repeating the input 4-8. The end of the model set-up is indicated by a card of type 4 with N = 0.

Card 9 **(P(I), I = 1,NP)** **[8F10.5]**

Other parameter sets may be considered by supplying additional cards of type 9.

B.8 Input for Program EFG

Card 1 **(IDIR(I), I = 1,10)** **[10I5]**

Card 2 **(Z(I), I = 1,MAXTYP)** **[8F10.6]**

Card 3 **DMAX** **[F10.6]**

Appendix C. Alphabetical List of Subroutines

The subroutines used in **GROUP**, developed by *WARREN* and *WORLTON*, are not included.

BL	stores the elements of the block diagonalized Dynamical Matrix into individual matrices.
BMP	calculates the force constants according to the Born-Mayer potential.
BOSE	calculates the Bose-factor n_{qj}.
CCF	calculates the (3 × 3) submatrices of Coulomb coefficients.
CHECKT	checks the translational invariance of the force constant matrix.
CINS	inserts complex (3 × 3) submatrices into a full (3N × 3N) matrix.
CMLIST	lists a complex matrix.
CMMULT	calculates the complex matrix product **A** = **B C**.
CMQ	equates two complex matrices.
CMZ	complex matrix zeroing routine
CP	calculates the Coulomb contribution to a (3 × 3) submatrix of the Dynamical Matrix.
CTOD	changes the Dynamical Matrix and related matrices from C- to D-definition.
CTRNSF	calculates the symmetrical equivalent submatrices of the Dynamical Matrix.
DIJ	calculates the complete (3 × 3) submatrices of the Dynamical Matrix.
DSF	calculates the dynamical structure factor for a particular phonon in a given Brillouin zone.
DWF	calculates Debye-Waller factors.
DYN2	constructs the entire Dynamical Matrix of dimension (3N × 3N).
EIGCH	diagonalizes a complex hermitian matrix (IMSL library routine).
EIGEN	calculates eigenvalues and eigenvectors of the Dynamical Matrix.
EMPTY	collects a string of characters which is needed for a histogram of dispersion curves.
EXTIP	extends the vector IP of parameter numbers in case of the shell model in order to account for the non-hermiticity of the matrix for the core-shell coupling.
FCCF	calculates the local electrical field.
FCM	calculates the (3 × 3) submatrix of the Dynamical Matrix on the basis of given longitudinal and transverse force constants.
FCP	calculates the local electrical field.
FREQ	transforms the eigenvalues of the Dynamical Matrix to frequency scale.
GETDT	reads the symmetry coordinates from file **COORD**.
GETPAR	interprets the user input for the model specification.

GETPM	gets the actual parameter values for a particular interaction by decoding the information contained in the vector IP.
GETTF	reads the temperature factors for one representative atom per atom type and calculates the temperature factors of symmetrical equivalent atoms.
GETXX	reads the atomic positions from file **COORD**.
HTRANS	calculates the hermitian matrix transformation $A = B^{+} C B$.
IMZ	integer matrix zeroing routine
INDINT	determines the total number of independent interactions.
IREP	determines the irreducible representation of modes which have been rearranged by subroutine SORT.
LENGTH	is a function and calculates the length of a N-dimensional vector.
LEQT1C	calculates the inverse of a complex matrix (IMSL library routine).
LINE	is a function and determines the print-line corresponding to a particular phonon wavevector within a histrogram plot.
LJP	computes force constants according to the Lennard-Jones potential.
MDM	multiplies the Dynamical Matrix by the mass-tensor.
MINS	inserts real (3×3) submatrices into the full force constant matrix.
MODELX	is called by SR DIJ and serves as a switch to a model potential number M.
MODX	represents an integer by a bit-pattern. MODX is used to determine which interaction types are superimposed for modelling a particular pair interaction.
MTRNSF	calculates symmetrical equivalent submatrices of the force constant matrix.
MZ	real matrix zeroing routine
NBR	analyzes the neighbourhood of a particular atom.
NPM	determines the number of atom-specific and interaction-specific parameters for a given model potential.
PCF	displays the pair correlation function as a histogram plot.
PDRV	calculates the partial derivates of phonon frequencies with respect to each of the model parameters.
PHASE	converts the Dynamical Matrix from D- to C-definition.
PRINT1	prints the model specification as the heading for an output list.
PRINT2	prints the results of model calculations.
PRINT3	prints the results of structure factor calculations.
PRINT4	prints the headings for structure factor output.
PRINT5	prints the headings for the results of structure factor calculations including the temperature factors and the scattering lengths.
PRINT6	prints the partial derivates of phonon frequencies.
RINV	checks the rotational invariance of a given lattice-dynamical model.
ROUND	zeroes those matrix elements whose moduli are smaller than a given amount.
RSTOR1	restores the parameters of model calculations from file **RESULT**.
RSTOR2	restores the results of model calculations from file **RESULT**.
SELF	calculates the self-term for the Dynamical Matrix and related matrices.

SHELL1 calculates the (3×3) submatrices for a particular pair interaction according to the shell model.

SHELL2 calculates the polarization part of the Dynamical Matrix according to the shell model.

SORT rearranges the elements of a real vector according to their moduli.

STOEIG stores eigenvalues and eigenvectors.

STORE1 stores the parameters of model calculations on file **RESULT**.

STORE2 stores the results of model calculations on file **RESULT**.

TYPE determines the number of different unit types of the given structure.

VDWP computes the force constants according to the van der Waals potential.

VPROD calculates the vector product $\mathbf{c} = \mathbf{a} \times \mathbf{b}$.

Appendix D. Subroutine Reference List

In the following, for each program of UNISOFT (except **GROUP**) the required subroutines are listed.

IND GETXX, INDINT, TYPE

NN EMPTY, GETXX, LENGTH, NBR, PCF

MODEL1 BL, BMP, CCF, CHECKT, CINS, CMLIST, CMMULT, CMQ, CMZ, CP,CTOD, CTRNSF, DIJ, DYN2, EIGCH, EIGEN, EXTIP, FCM, GETDT, GETPAR, GETPM, GETXX, IMZ, HTRANS, LENGTH, LEQT1C, LJP, MDM, MINS, MODELX, MODX, MTRNSF, MZ, NPM, PRINT1, PRINT2, ROUND, SELF, SHELL1, SHELL2, STOEIG, STORE1, STORE2, VDWP

HIST EMPTY, GETXX, LENGTH, LINE, MODX, PRINT1, RSTOR1 RSTOR2, VPROD

SF BOSE, DSF, DWF, FREQ, GETTF, GETXX, IREP, LENGTH, MODX, PRINT3, PRINT4, PRINT5, RSTOR1, RSTOR2, SORT

PARDER BMP, CCF, CINS, CMZ, CP, CTOD, CTRNSF, DIJ, DYN2, FCM, FREQ, GETDT, GETPM, GETXX, HTRANS,IMZ LENGTH, LEQT1C, LJP, MDM, MINS, MODELX, MODX, MTRNSF, MZ, PDRV, PRINT1, PRINT6, ROUND, SELF, SHELL1, SHELL2, RSTOR1, RSTOR2, VDWP

ROTINV BMP, CCF, CINS, CMLIST, CMZ, CP, CTOD, CTRNSF, DIJ, DYN2, EXTIP, FCM, GETPAR, GETPM, GETXX, IMZ, HTRANS, LENGTH, LEQT1C, LJP, MDM, MINS, MODELX, MODX, MTRNSF, MZ, NPM, PHASE, PRINT1, RINV, ROUND, SELF, SHELL1, SHELL2, VDWP

EFG CCF, CMZ, CP, FCCF, FCP, GETXX, MZ

Appendix E. List of Symbols

As a general convention, bold printed capital letters are used to denote matrices, while bold printed lower case letters represent vectors.

a_{qj}	annihilation operator for a phonon state qj
a_{qj}^{-}	creation operator for a phonon state qj
$\mathbf{B}_\kappa$	matrix of temperature factors of atom κ
b_κ	scattering length of atom κ
$\mathbf{C}(q)$	matrix of Coulomb coefficients at wavevector q
$\mathbf{C}(\kappa\kappa'\|q)$	(3 × 3) submatrix of C(q)
$\mathbf{D}(q)$	Dynamical Matrix at wavevector q
$\mathbf{D}^X$	block diagonalized Dynamical Matrix
$\mathbf{D}(\kappa\kappa'\|q)$	(3 × 3) submatrix of D(q)
$\mathbf{D}^{(m)}(\kappa\kappa'\|q)$	contribution of interaction type m to $\mathbf{D}(\kappa\kappa'\|q)$
d_n	radius of the n-th neighbouring shell
$\mathbf{E}$	matrix of eigenvectors
$\mathbf{e}(qj)$	eigenvector of the Dynamical Matrix corresponding to the phonon state qj
$\mathbf{e}_i^X$	eigenvector of the block diagonalized Dynamical Matrix
$\mathbf{e}(\kappa\|qj)$	eigenvector of atom κ corresponding to the phonon state qj
erf	error function
e^{-W_κ}	Debye-Waller factor of atom κ
$\mathbf{F}(q)$	Fourier transformed force constant matrix at wavevector q
$\mathbf{F}(\kappa\kappa'\|q)$	(3 × 3) submatrix of F(q)
$\mathbf{F}^C(q)$	Coulomb part of F(q)
$\mathbf{F}^C(\kappa\kappa'\|q)$	(3 × 3) submatrix of $\mathbf{F}^C(q)$
$\mathbf{F}^{CC}$	Fourier transformed force constant matrix for the *effective* core-core coupling
$\mathbf{F}^{CS}$	Fourier transformed force constant matrix for the *effective* core-shell coupling
$\mathbf{F}^S(q)$	Fourier transformed force constant matrix for the shell-shell coupling
$\mathbf{F}^S(\kappa\kappa'\|q)$	(3 × 3) submatrix of $\mathbf{F}^S(q)$
$\mathbf{F}^{SC}$	Fourier transformed force constant matrix for the *effective* shell-core coupling
$\mathbf{F}^{SS}$	Fourier transformed force constant matrix for the *effective* shell-shell coupling
$\mathbf{F}^T(q)$	Fourier transformed force constant matrix for the core-shell coupling
$\mathbf{F}_0^T$	matrix of the self terms of $\mathbf{F}^T(q)$
$\mathbf{F}^T(\kappa\kappa'\|q)$	(3 × 3) submatrix of $\mathbf{F}^T(q)$
$\mathbf{F}^{T'}(q)$	Fourier transformed force constant matrix for the shell-core coupling
$\mathbf{F}_0^{T'}$	matrix of the self terms of $\mathbf{F}^{T'}(q)$
$\mathbf{F}^{T'}(\kappa\kappa'\|q)$	(3 × 3) submatrix of $\mathbf{F}^{T'}(q)$
$\mathbf{F}^{(m)}(\kappa\kappa'\|q)$	contribution of interaction type m to $\mathbf{F}(\kappa\kappa'\|q)$
$f_\alpha^\beta(\kappa l)$	α-component of the force acting upon an atom (κl) during a rigid rotation of the whole crystal around the β-axis
g	reciprocal lattice vector
G	order of a symmetry group
g	element of a symmetry group
G_q	symmetry group of the wavevector q
$\mathbf{H}$	tensor of electrical field gradients
$\mathbf{h}$	local electrical field
h	Planck constant ($6.626\ 10^{-34}$ Js)
$\hbar$	$h/2\pi$ ($1.055\ 10^{-34}$ Js)
H	Hamiltonian
H_{qj}	Hamiltonian for one particular phonon state qj
$\hbar\omega$	energy transfer in neutron scattering experiments
$\mathbf{I}$	unit matrix
$\mathbf{K}$	diagonal matrix of intraatomic core-shell force constants
K_κ	core-shell force constant within the same atom κ
k_B	Boltzmann constant ($1.381\ 10^{-23}$ JK^{-1})

$\mathbf{k}_i$, $\mathbf{k}_j$	neutron wavevectors
L	longitudinal force constant
l,l',m,m'	label different primitive cells
M	mass-tensor
m_κ	mass of atom κ
m_n	neutron mass
N	number of atoms per primitive cell
n_{qj}	Bose-factor corresponding to the phonon state **qj**
p	parameter vector corresponding to a particular model
$\Delta\mathbf{p}$	variation of **p**
$\mathbf{p}_{\kappa l}$	momentum of atom (κl)
$\mathbf{p}^e_{\kappa l}$	electric dipole moment of atom (κl)
p	parameter for the Ewald-summation
Q	scattering *vector* (the only exception from the above convention)
q	phonon wavevector
$\delta\mathbf{q}$	small increment of **q**
δq	modulus of $\delta\mathbf{q}$
qj	phonon state
Q_{qj}	normal coordinate corresponding to the phonon state **qj**
r	vector in real space
r	modulus of vector **r**
$\mathbf{r}_{\kappa l}$	position vector of atom (κl)
$\mathbf{r}^o_{\kappa l}$	equilibrium position of atom (κl)
S	rotational matrix corresponding to a symmetry operation
(**S**|**v**)	symmetry operation
$S_{coh}(\mathbf{Q}, \omega)$	coherent scattering function
$S^{(qj)}_{coh}(\mathbf{Q}, \omega)$	coherent scattering function due to the interaction of a neutron with a single phonon state **qj**
T	transverse force constant
T	temperature
t	time variable
$TF_\kappa(i)$	component of the tensor of temperature factors $\mathbf{B}_\kappa$
$\mathbf{u}_{\kappa l}$	displacement vector of atom (κl)
$\mathbf{V}(\kappa l, \kappa' l')$	force constant matrix for the interaction between atoms (κl) and (κ'l')
$\mathbf{V}^S(\kappa l, \kappa' l')$	force constant matrix for the shell-shell interaction between atoms (κl) and (κ'l')
$\mathbf{V}^{SR}(\kappa l, \kappa' l')$	force constant matrix for the short-range core-core interaction between atoms (κl) and (κ'l')
$\mathbf{V}^T(\kappa l, \kappa' l')$	force constant matrix for the core-shell interaction between atoms (κl) and (κ'l')
$\mathbf{V}^{T'}(\kappa l, \kappa' l')$	force constant matrix for the shell-core interaction between atoms (κl) and (κ'l')
v	fractional translation of a symmetry operation
$V(\kappa l, \kappa' l')$	potential energy due to the interaction between atoms (κl) and (κ'l')
V_o	prefactor for model potentials
v	volume of the primitive cell
$\mathbf{w}_{\kappa l}$	displacement vector of the electron shell of atom (κl) with respect to its equilibrium position
$\bar{\mathbf{w}}_{\kappa l}$	relative displacement vector of the electron shell of atom (κl) with respect to corresponding core-position
X	matrix of symmetry coordinates
X_κ	charge of the ionic core of atom κ
Y	matrix of shell charges
Y_κ	charge of the electron shell of atom κ
Z	matrix of ionic charges
Z_κ	charge of ion κ
α_κ	polarizability of the free ion κ
Γ_{3N}	3N-dimensional representation of a symmetry group
γ_i	irreducible multiplier representation no. i
$\delta_{\alpha,\beta}$	Kronecker-symbol
ε_o	vacuum permittivity ($8.854\ 10^{-12}$ As(Vm)$^{-1}$)
κ, κ', λ, λ'	label atoms within a primitive cell
ν_{qj}	$= \omega_{qj}/2\pi$, frequency of the phonon state **qj**
Δν	variation of frequency ν

$\delta\nu^2$	variation of squared frequency ν^2
ρ_κ	charge distribution representing the ion κ
Σ	sum
σ_κ	short range repulsion parameter of atom κ
χ	character of a representation
ω_{qj}	frequency of the phonon state qj
$\Delta\omega$	variation of the frequency ω
$\delta\omega^2$	variation of the squared frequency ω^2
$*$	complex conjugate
$+$	hermitian conjugate